Pollution Prevention

(P2) Framework

U.S. Environmental Protection Agency

Office of Pollution Prevention and Toxics

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Disclaimers

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The models presented in OPPT's P2 Framework have been developed over a period of more than 20 years by OPPT, EPA contractors and/or grantees or others in the scientific and technical community, to screen chemicals in the absence of data. Through the P2 Framework, OPPT is presenting these screening models to industry and other stakeholders in the hopes that use of these models early in the research and development process will result in safer chemicals entering commerce. The P2 Framework models should be used to provide additional information on chemicals of concern.

Other chemical screening methodologies have been developed and are in use by chemical companies and other stakeholders. The Agency recognizes that other models are available and that these models can also be of value in chemical screening efforts.

CAUTION: Screening models predict data with an inherent degree of uncertainty, and should *never* be used to replace measured data from well designed studies. Measured data are always preferred over predicted data. If measured data are not available, measured data on close analogs can be used. If no analog data are available, screening level models, such as those in the P2 Framework, may be used to predict values that can be used to indicate which chemicals may need further testing.

Contents

*Definitions of terms in italics are provided in the Glossary.

Contents (continued)

The Pollution Prevention (P2) Framework
Developed by:
The Office of Pollution Prevention and Toxics
U.S. Environmental Protection Agency

Executive Summary

Of the approximately 80,000 chemicals used in commerce in the United States, few have been tested, and only a fraction have sufficient information to allow a thorough evaluation of risk. Businesses, governmental organizations, and other stakeholders often don't have the data necessary to identify problem chemicals or identify safer substitutes or other options that are less risky, prevent pollution, and may save companies environmental management costs. At times, companies must make product and process decisions without enough data regarding the risk tradeoffs.

The Office of Pollution Prevention and Toxics (OPPT) has developed computer-based methods that derive important risk assessment information based on chemical structure and other factors. These methods provide information on physical / chemical properties, environmental fate, potential *carcinogenicity*, toxicity to aquatic organisms, worker and general population exposures, among other data. OPPT routinely uses these methods to highlight chemicals of concern, to identify safer substitutes, and to reduce or eliminate risks.

The Pollution Prevention Framework ("P2 Framework") is a document that contains many of OPPT's most important computer-based methods for assessing risk. The P2 Framework provides important risk-related tools not previously available. Its purpose is to provide information that can inform decision making and help promote the design, development, and application of safer chemicals and processes. The document describes each assessment methodology and the importance of the data generated, and provides case studies showing how methods can be used collectively to answer complicated risk assessment questions and identify pollution prevention opportunities. The P2 Framework, as currently constructed, does not address all biological endpoints. It is a set of screening-level methods that are of most value when chemical-specific data are lacking.

What Is Pollution Prevention?

"Pollution prevention" is the common sense understanding that it is easier to prevent problems than to correct them. Congress, by enacting the Pollution Prevention Act of 1990 (42 U.S.C. 13101 and13102, s/s et seq.), created a bold national objective for environmental protection by outlining a hierarchy in dealing with pollution:

✓ Pollution should be prevented or reduced at the source whenever feasible;

✓ Pollution that cannot be prevented should be recycled in an environmentally safe manner whenever feasible;

✓ Pollution that cannot be prevented or recycled should be treated in an environmentally safe manner whenever feasible; and

✓ Disposal or other releases into the environment should be employed only as a last resort and should be conducted in an environmentally safe manner.

Pollution prevention means "source reduction," as defined under the Pollution Prevention Act.   The Pollution Prevention Act defines "source reduction" to mean any practice which:

✓ Reduces the amount of any hazardous substance, pollutant, or contaminant entering any waste stream or otherwise released into the environment prior to recycling, treatment, or disposal; and

✓ Reduces the hazards to public health and the environment associated with the release of such substances, pollutants, or contaminants.

Source reduction can be achieved through equipment or technology modifications, processes or procedure modification, reformulation or redesign of products, substitution of materials, etc.

Pollution Prevention in the
Industrial and Commercial Chemicals Sector:
Risk Information Improves Decision Making

Approximately 80,000 different chemicals are commercially available in the United States. An additional 1,500 - 2,000 new chemicals per year are evaluated by EPA's Office of Pollution Prevention and Toxics (OPPT) . Relatively few have been tested, and only a fraction have sufficient information to allow a thorough evaluation of risk. Businesses, governmental organization and other stakeholders may not have the data necessary to identify problem chemicals or identify substitutes or options that are less risky, prevent pollution, and may be less costly in terms of environmental management. At times, some companies must make product and process decisions without data regarding the risk tradeoffs.

To identify and take advantage of pollution prevention opportunities, stakeholders need access to risk-related information. Companies often decide which chemicals or processes to use primarily on the basis of cost and product performance, among other criteria. If companies had access to risk-related information about chemicals, they could improve decision making and take advantage of pollution prevention opportunities.

A generalized example might help illustrate how risk-related information can drive pollution prevention outcomes. Company A plans to formulate a concentrated, heavy duty industrial cleaner, and needs to incorporate a solvent within the product to meet the customer's performance criteria. Twelve solvents are available that all meet the customer's performance and cost criteria. The company knows the chemical is likely to be discharged to water, and is concerned about toxicity to aquatic life. The company decides to test each of the 12 solvents for three parameters: (1) persistence in the environment, (2) *bioconcentration*, and (3) fish *acute toxicity*. The test results are summarized as follows:

Seven of the 12 solvents showed:
  ✓ very low *bioconcentration* potential
  ✓ rapid degradation
  ✓ low aquatic toxicity

Five of the 12 solvents showed:
  ✓ high *bioconcentration* potential
  ✓ persistence in the environment for
    several months
  ✓ moderate to high fish *acute toxicity*

Pollution Prevention in the Industrial and Commercial Chemicals Sector: Risk Information Improves Decision Making (continued)

Testing indicates that 5 of the 12 solvents raise significant pollution and toxicity concerns. As a result, the company chose one of the seven solvents with low *bioconcentration* potential, a high degradation rate, and low aquatic toxicity. In this example, price and product performance characteristics of potential solvents were equivalent, and it was risk-related information that led to a clear pollution prevention outcome.

The P2 Framework

EPA's Office of Pollution Prevention and Toxics (OPPT) has developed computer-based methods that derive important risk assessment information, such as the information discussed in the above example. OPPT routinely uses these methods to highlight chemicals of concern, evaluate the relative safety of substitute chemicals, and identify opportunities for reducing or eliminating risk. The P2 Framework is a compilation of some of OPPT's most important methods for assessing risk when chemical specific data are lacking. This document describes each assessment methodology contained in the P2 Framework and the importance of the data generated for decision making. This document also includes case studies showing how methods can be used collectively to answer complicated risk assessment questions and identify P2 opportunities.

The P2 Framework provides important risk assessment information not previously available. The purpose of the P2 Framework is to help identify pollution prevention opportunities by providing information that can inform decision making and help promote the design, development and application of safer chemicals and processes.

The Risk Assessment Process

In 1983, the National Academy of Sciences developed a 4 step paradigm for risk assessment and risk management*:

✓ *Hazard* Identification: Examining toxicity data to determine effects of a chemical on health of humans or other organisms (for example, increased cancer cases or birth defects);

✓ Dose-Response Assessment: Extrapolating toxicity data from high *dose* studies to predict the likely effect of low doses of the chemical (also referred to as *Hazard* Characterization);

✓ Exposure Assessment: Magnitude, frequency, and duration of exposure to a chemical (for example, exposures from proposed or actual manufacture, use, or disposal of a chemical); and

✓ Risk Characterization: Estimates potential for, and magnitude of, risk to an exposed individual or population.

The components of the risk assessment process are illustrated in the following figure:

The Risk Assessment Paradigm

| Hazard Identification | → | Dose-Response Assessment |
| Exposure Assessment | → | Risk Characterization |
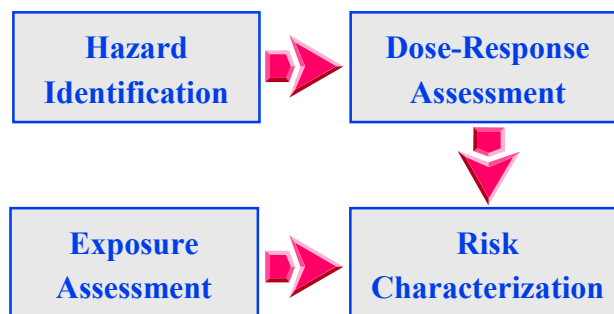
*NRC. 1983. Risk Assessment in the Federal Government: Managing the Process. National Research Council. National Academy Press, Washington, DC.

How Do These Methods Help the Risk Assessor?

P2 Framework Methods Help Assess Risk of a Chemical

Most methods presented in OPPT's P2 Framework deal with two steps of the risk assessment process: *hazard* identification and exposure assessment. Ideally, information on the potential hazards posed by a chemical as well as exposure information will be available, but often this is not the case. Methods included in the P2 Framework are intended to provide information to help in assessing potential risk posed by a chemical or group of chemicals.

What to Do When There Are No Data

The methods are intended to be used when data are unavailable or to supplement available data. These methods are generally computer models that assess a particular aspect of a chemical's possible impact on humans or the environment. For example, one model estimates toxicity to fish, aquatic invertebrates, and algae. This is important information if the chemical is or will be discharged to streams during manufacture, processing, use, or disposal. The OncoLogic model estimates the likelihood that a chemical would cause cancer in humans. Other models estimate potential exposures to a chemical in consumer products. Models are also presented for estimating properties such as vapor pressure and water solubility, which are important for projecting the nature, magnitude, and duration of exposure.

These Methods Provide Information in Four Areas

The P2 Framework provides information in the following areas:

Physical/Chemical Properties
✓ Melting point
✓ Boiling point
✓ Vapor pressure
✓ Water solubility
✓ Organic carbon adsorption
✓ Henry's law constant

Chemical Fate in the Environment
✓ Atmospheric oxidation potential
✓ Biodegradation
✓ Hydrolysis
✓ *Bioconcentration*
✓ Percent removal in wastewater treatment

***Hazard* to Humans and the Environment**
✓ *Carcinogenicity* potential
✓ *Aquatic toxicity*

Exposure and/or Risk
✓ Consumer dermal exposure
✓ Consumer inhalation exposure
✓ Stream concentrations and human potential *dose* rates from discharges to surface water
✓ *CC* exceedences from discharges to surface water
✓ Occupational exposure for several scenarios

The P2 Framework is set of screening-level methodologies that can be used when chemical-specific data are lacking. **If data are available for a given endpoint from a well conducted test, they should be used instead of data generated by the P2 Framework models or similar screening-level models.** The P2 Framework, as currently constructed, does not address all human health or ecological effects. For example, methods are lacking to predict reproductive toxicity, developmental toxicity, and neurotoxicity, among others. Some methods included in the P2 Framework provide quantitative estimates (e.g., methods to estimate aquatic toxicity), while others, such as the OncoLogic model, provide qualitative *hazard* estimates.

What is Required to Use the P2 Framework Models?

Essential Information

All of the tools require minimal, but important information. For example, physical and chemical properties such as molecular weight are important. Other models require the user to input the amount of chemical likely to be discharged to a stream or river. The table on the following page summarizes the required input information as well as the output data for each model.

Knowledge or Expertise Required

Knowledge needed will vary depending on the application. For example, the models KOWWIN and PCKOCWIN only require chemical structure or *CAS Number*; however, ECOSAR and OncoLogic require that the user have a good understanding of organic chemistry. User's Guides and technical assistance are available to help when you are uncertain how to proceed.

Model Availability

Models to Estimate Physical/Chemical Properties of Chemicals:
MPBPVP, KOWWIN, WSKOW, PCKOCWIN, HENRYWIN, and BCFWIN methods were developed by Syracuse Research Corporation (SRC) under contract to US EPA, OPPT in support of Section 5 of TSCA, and are available from SRC, Syracuse, N.Y., 6225 Running Ridge Rd., North Syracuse, NY 13212.

Models to Estimate Chemical Fate in the Environment:
AOPWIN, BIOWIN, HYDROWIN, and STPWIN methods were developed by SRC under contract to US EPA, OPPT in support of Section 5 of TSCA, and are available from SRC.

Models to Estimate *Hazard* to Humans and the Environment:
OncoLogic, developed by LogiChem under a cooperative agreement with USEPA, OPPT in support of Sec. 5 of TSCA, can be obtained by contacting: Marilyn S. Arnott, Ph.D., LogiChem, Inc., PO Box 622, Narberth, PA 19072, Email: marnott@ptdprolog.net
ECOSAR can be obtained by downloading from the Internet at: http://www.epa.gov/oppt/newchems/21ecosar.htm or by contacting Vince Nabholz, EPA, OPPT at nabholz.joe@epa.gov

Models to Estimate Exposure and/or Risk:
The E-FAST Model and documentation manual can be downloaded at no cost from the Internet at: http://www.epa.gov/opptintr/exposure
ReachScan can be obtained by contacting Tom Brennan, EPA, OPPT at brennan.thomas@epa.gov
Occupational Exposure Spreadsheets can be obtained by contacting Scott Prothero, EPA, OPPT at prothero.scott@epa.gov

The computer "Wizard"

Computer Requirements

These models are designed to run on IBM compatible personal computers. The specific computer requirements (memory and disk size) necessary to run each of these models vary and are provided in a later section of this manual.

Inputs and Outputs of the P2 Framework Models

Models to Estimate Physical / Chemical Properties

Model	Output	Input
MPBPVP	Melting and Boiling Points, Vapor Pressure	CAS No. or Chem. Str. In SMILES
KOWWIN	Octanol / water partition coefficient	CAS No. or Chem. Str. In SMILES
WSKOW	Water solubility from log KOW	CAS No. or Chem. Str. In SMILES
PCKOCWIN	Soil organic carbon partition coefficient	CAS No. or Chem. Str. In SMILES
HENRYWIN	Henry's law constant: VP/WS	CAS No. or Chem. Str. In SMILES
BCFWIN	*Bioconcentration* factor	CAS No. or Chem. Str. In SMILES

Models to Estimate Chemical Fate in the Environment

Model	Output	Input
AOPWIN	Atmospheric oxidation potential	CAS No. or Chem. Str. In SMILES
BIOWIN	Biodegradation rate	CAS No. or Chem. Str. In SMILES
HYDROWIN	Hydrolysis rate	CAS No. or Chem. Str. In SMILES
STPWIN	Percent removal in POTW	CAS No. or Chem. Str. In SMILES

Models to Estimate *Hazard*s to Humans and the Environment

Model	Output	Input
OncoLogic	Cancer *hazard* potential	Chemical structure
ECOSAR	*Acute* and *Chronic toxicity* to fish, invertebrates, algae	CAS No. or Chem. Str. In SMILES

Models to Estimate Exposure and / or Risk

Model	Output	Input
E-FAST	Surface water ingestion, fish ingestion, ground water ingestion, ambient air inhalation, indoor air inhalation, dermal exposure, aquatic environment exposure/risk	Physical / chemical properties, fate properties, release amounts, release medium, release location, aquatic concentration of concern, *NPDES* number
ReachScan	Impact of surface water discharges on drinking water facilities, chemical concentration downstream at drinking water intake point	Facility location(*NPDES*), release data
Occupational Exposure Spreadsheets	Vapor generation rates and worker exposure to vapors during filling, sampling, and to open liquid pools; and during degreasing operations; water releases and worker exposures to powders during textile dyeing	Molecular weight, vapor pressure, operation hrs/day, worker exposure hrs/day; if applicable volume of degreasing solvent or dye used, dye exhaust rate

About This Document

Contents of This Document

This manual explains the models used by OPPT to screen potential exposures and risks posed by chemicals. Each model answers important questions about a chemical's potential impact on humans or the environment. The models are described in this document by briefly detailing the important information they provide. Flow diagrams presenting step-by-step use of some of the more complex models are also included. In addition, a series of structured examples (case studies) are provided to show how the models can answer specific environmental questions and how the models can be used in combination to answer complicated exposure/risk-related questions.

We believe this information will be useful to you. The manual provides some information on how to use the models. However, we recognize that you may still have questions after you read this material. Technical assistance is available from OPPT to answer those questions.

Users of This Document

You are reading this manual because you are interested in opportunities to prevent pollution. These opportunities may also decrease costs to your company or organization. As you read, please keep in mind that this version of the P2 Framework is the first step in an evolving process. All comments and suggestions for improvement are welcome. Please direct comments to:

>   Maggie Wilson, EPA/OPPT
>   Phone: 202-260-3902
>   Email: wilson.maggie@epa.gov

How This Document Is Organized

This document presents brief overviews of 18 models. Each overview provides enough information to successfully run each model. More detailed information on each model is provided in the User's Guide or supplemental documentation for that model.
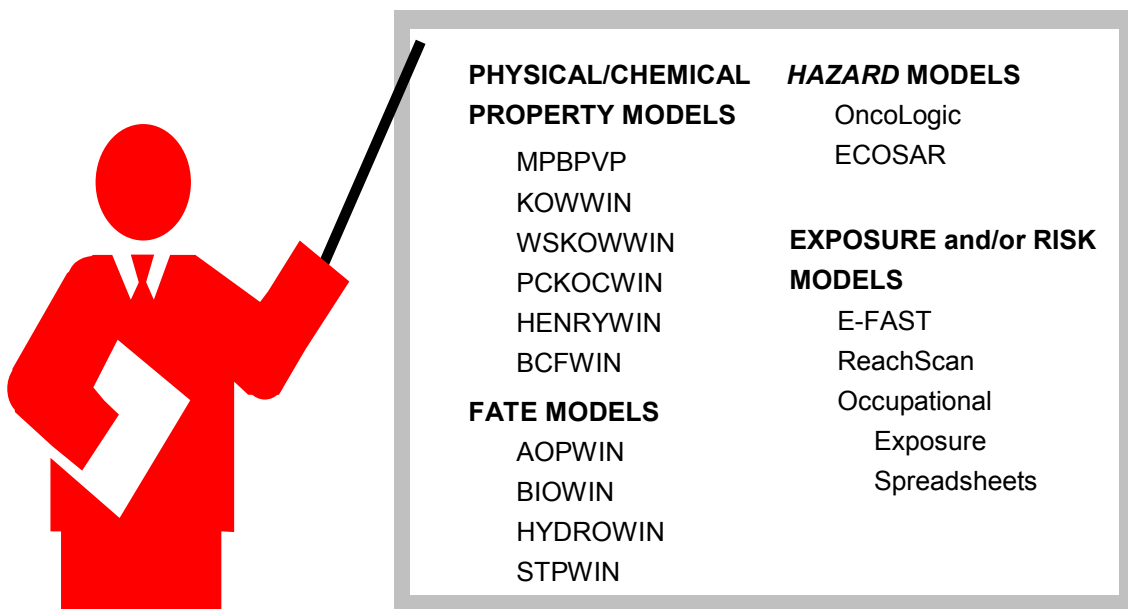
A glossary of relevant terms is also included. Terms in the text of the document that appear in *italics* are defined in the glossary.

Appendices include (1) Case Studies which illustrate how the models can be used in combination to answer complicated risk-related questions; (2) Data Sources to search for measured data; (3) and Summary of Writing SMILES notation.

Models Presented

The models included in this manual are listed below, and
are presented in the illustration on the following page.
The illustration can be used as an informal "road map" to
help decide which models you will need to use.

**PHYSICAL/CHEMICAL
PROPERTY MODELS**
- MPBPVP
- KOWWIN
- WSKOWWIN
- PCKOCWIN
- HENRYWIN
- BCFWIN

FATE MODELS
- AOPWIN
- BIOWIN
- HYDROWIN
- STPWIN

***HAZARD* MODELS**
- OncoLogic
- ECOSAR

**EXPOSURE and/or RISK
MODELS**
- E-FAST
- ReachScan
- Occupational
  Exposure
    Spreadsheets

P2 Framework Models

AOPWIN

MPBPVPWIN

Occupational**

STPWIN

OncoLogic

WSKOWWIN

PCKOCWIN

HENRYWIN

E-FAST*

ReachScan

BIOWIN

HYDROWIN

BCFWIN

ECOSAR

KOWWIN

*Incorporates SCIES, Dermal, SEAS, and PDM3
** Being migrated to Windows-based ChemSTEER

EPIWIN and SMILES

What Is EPIWIN?

Estimations Programs Interface for Windows (EPIWIN) provides a quick and easy way to run the estimation programs, listed below, from a single entry for a single chemical. The chemical structure or *CAS Number* is entered only once, and EPIWIN executes all of the programs in sequence and captures their output. Any of the estimation programs may be run separately. The EPIWIN Programs also can input chemical structure formats generated by other computer programs. These importable formats include:

Alchemy III MOL files	HyperChem HIN files	PCModel files
Beilstein ROSDAL files	MDL ISIS SKC files	Softshell SCF files
BioCAD Catalyst TPL files	MDL MOL files	Tripos Sybyl Line Notation
ChemDraw files	Molecular Presentation	Tripos SYBYL MOL2 files
ChemDraw Connection Tables	Graphics MPG files	

The computer "Wizard"

EPIWIN Can Sequentially Run:

✓ AOPWIN
✓ BCFWIN
✓ BIOWIN
✓ ECOSAR
✓ HENRYWIN
✓ HYDROWIN
✓ KOWWIN
✓ MPBPVP
✓ PCKOCWIN
✓ STPWIN
✓ WSKOW

What Is SMILES?

SMILES is "Simplified Molecular Input Line Entry System," which translates a chemical's structure into a string of symbols that is easily understood by computer software. You can learn to write SMILES notations, as described in Appendix C. For all EPIWIN estimation programs, enter only the SMILES notation for the chemical, and the program provides the estimation you need.

SMILES Notations
(Examples Provided in Appendix C)

Writing SMILES Notations

The SMILES notation system was designed by chemists for computer use (Weininger, 1988. J. Chem. Inf. Comput. Sci. 28: 31-6). SMILES notations depict the molecular structure of a chemical as a 2-dimensional picture. Learning to write a SMILES notation is not difficult, but it can be tricky. The same 3-dimensional structure can be written correctly using many different SMILES notations.

The rules for writing SMILES notations are included in the EPIWIN User's Guide available from Syracuse Research Corporation (SRC); however, you can purchase the SMILECAS data base from SRC that contains SMILES notations of many chemicals.

Some Rules for Writing SMILES Notations

Atoms are represented by atomic symbols. *Aliphatic* atoms are entered in upper case, and *aromatic* atoms (carbon, oxygen, sulfur, selenium, and nitrogen) are entered in lower case. Examples:

Ethane (CH_3-CH_3)	CC
Benzene (C_6H_6)	c1ccccc1
Ethylbenzene ($C_6H_5C_2H_5$)	CCc1ccccc1
Bromoethane (CH_3-CH_2-Br)	CCBr
1,3-Dichloropropane (CL-CH_2-CH_2-CH_2-CL)	CLCCCCL

Four types of Bonds are represented in SMILES. These include:
- Single Bonds* -- represented by a hyphen "**-**". However, the program drops the hyphen, so it is not necessary to type it. Ethane (CH_3-CH_3) is CC and not C-C.
- Double Bonds -- represented by an equal "**=**" and must be indicated. Ethylene (CH_2=CH_2) is C=C.
- Triple Bonds -- represented by a number symbol "**#**", for example acetylene (CH_2≡CH_2) is C#C.
- Aromatic Bonds* -- represented by a "**:**", and are indicated by lower case.

*Normally single bonds and aromatic bonds do not need to be written in the SMILES notation.

Branches are designated in enclosed parentheses, for example 2-Propanol is CC(O)C. Branches can not begin a SMILES notation and must follow the atom and not the bond symbol.

Cyclic Structures are the most complicated to write. Numbers (1-9) are used to indicate where the ring starts and stops, and never follow a branch.

A summary of directions for writing SMILES notations is included in Appendix C of this document. Complete directions for writing SMILES notations are included in the EPIWIN User's Guide, and the Help files in each EPIWIN and the ECOSAR models included examples of SMILES notations.

Models to Estimate
Physical/Chemical Properties of Chemicals

Following are brief fact sheets providing information on the
models OPPT uses to estimate physical and chemical properties
of chemicals. Information provided on each model includes:

- ✓ What physical/chemical property does the model
  estimate?

- ✓ What is significant about the physical/chemical property
  to risk assessment?

- ✓ Why is knowing physical/chemical properties important?

- ✓ Why would I want to use the model?

- ✓ What do I need to run the model?

- ✓ What are the inputs and outputs for the model?

**PHYSICAL/CHEMICAL
PROPERTY MODELS**
  MPBPVP
  KOWWIN
  WSKOWWIN
  PCKOCWIN
  HENRYWIN
  BCFWIN
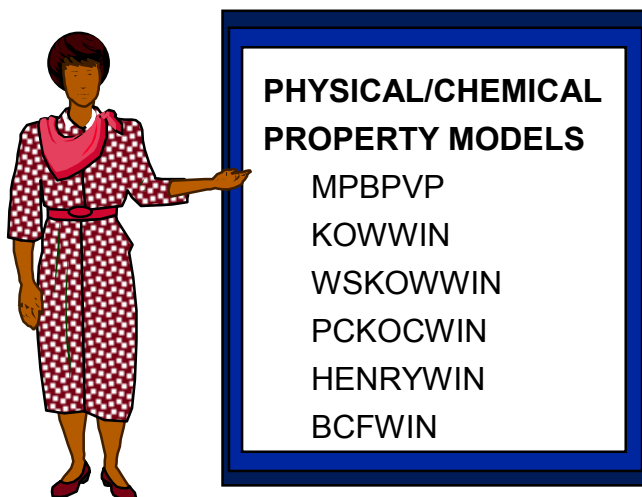
Notes

MPBPVP to Estimate
Melting Point, Boiling Point, and Vapor Pressure

Why is Melting Point (MP) Important?

MP is temperature at which a chemical changes from solid to liquid, and gives clues to other chemical properties:

✓ MP indicates state (solid-liquid-gas) of the chemical in the ambient environment.

✓ High MP indicates low water solubility.

✓ Low MP indicates increased absorption is possible through the skin, GI tract, or lungs.

✓ The range of measured MPs indicates it purity: narrow = more pure, wide = less pure.

✓ MP <100°C = increased volatility and higher potential exposures.

Why Use the MPBPVP Model?

> I need to know if the chemical is most likely to be a solid, liquid, or gas in the ambient environment, and at what temperature it will change phases.

Phase Changes

What Does the MPBPVP Model Do?
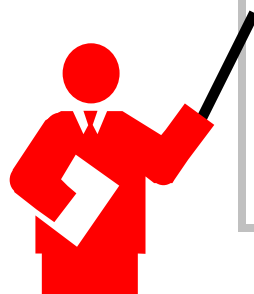
> MPBPVP estimates a chemical's melting point, boiling point, and vapor pressure at 25°C.

Why is Boiling Point (BP) Important?

BP is the temperature at which the VP of a chemical in a liquid state equals atmospheric pressure, and, like MP, gives clues to other chemical properties:

✓ High BP indicates low VP, for example structurally large substances like polymers.

Why is Vapor Pressure (VP) Important?

VP is pressure at which a liquid and its vapor are in equilibrium at a given temperature, and, like MP and BP, gives clues to other chemical properties:

✓ Chemicals with VP $\geq 10^{-4}$ mm Hg (higher VP) exist mostly in the vapor phase, and often have higher potential inhalation exposures than chemicals with low vapor pressure.

✓ Chemicals with VP 10^{-5} to 10^{-7} mm Hg exist in both vapor and particulate phases.

✓ Chemicals with (lower VP) $\leq 10^{-8}$ mm Hg exist mostly as particulates.

MPBPVP to Estimate
Melting Point, Boiling Point, and Vapor Pressure

What You Need to Use MPBPVP

✓ *CAS number* or chemical structure in SMILES

Inputs

✓ *CAS number* or chemical structure in SMILES notation

Examples of Melting Points at 25º C

CAS Number	Chemical	Degrees C
60571	Dieldrin	135
108952	Phenol	-2
75092	Dichloromethane	-90
67641	Acetone	-94
50000	Formaldehyde	-111

Examples of Boiling Points at 25º C

CAS Number	Chemical	Degrees C
60571	Dieldrin	340
108952	Phenol	170
75092	Dichloromethane	80
67641	Acetone	45
50000	Formaldehyde	10

Examples of Vapor Pressures at 25º C

CAS Number	Chemical	mm Hg@25C
50000	Formaldehyde	1330
67561	Methanol	396
75092	Dichloromethane	86
108952	Phenol	1
60571	Dieldrin	1.77E-5

Outputs

✓ Molecular weight and formula

✓ Estimations of melting point, boiling point, and vapor pressure at 25°C

✓ Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Saving Output

Output files can be saved as a ".dat" file or copied through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard.

Sample Output from the MPBPVP Model

INPUTS:

CAS Number = 108883 (Methyl-benzene or toluene)

RESULTS:

```
SMILES : c(cccc1)(c1)C
CHEM   : Benzene, methyl-
MOL FOR: C7 H8
MOL WT : 92.14
---------------- SUMMARY MPBPWIN v1.40 --------------
Boiling Point:  125.72 deg C (Adapted Stein and Brown

Melting Point:  -78.09 deg C (Adapted Joback Method)
Melting Point:  -40.26 deg C (Gold and Ogle Method)
Mean Melt Pt :  -59.17 deg C (Joback; Gold,Ogle Methods)
  Selected MP:  -59.17 deg C (Mean Value)

Vapor Pressure Estimations (25 deg C):
  (Using BP: 110.60 deg C (exp database))
  (MP not used for liquids)
    VP:  25.1 mm Hg (Antoine Method)
    VP:  22.3 mm Hg (Modified Grain Method)
    VP:  29.2 mm Hg (Mackay Method)
  Selected VP:  23.7 mm Hg (Mean of Antoine & Grain methods)
```

Melting point is calculated by two different methods, mean value is determined, and the mean is selected as the melting point.

Vapor pressure also is calculated by two different methods, and a mean value is selected as the vapor pressure.

```
-------+-----+--------------------+----------+---------
 TYPE  | NUM | BOIL DESCRIPTION   |  COEFF   |  VALUE
-------+-----+--------------------+----------+---------
 Group |  1  | -CH3               |   21.98  |   21.98
 Group |  5  | CH (aromatic)      |   28.53  |  142.65
 Group |  1  | -C (aromatic)      |   30.76  |   30.76
   *   |     | Equation Constant  |          |  198.18
============+====================+==========+=========
RESULT-uncorr|  BOILING POINT in deg Kelvin |  393.57
RESULT- corr |  BOILING POINT in deg Kelvin |  398.88
             |  BOILING POINT in deg C      |  125.72
-----------------------------------------------------
-------+-----+------------------+----------+---------
 TYPE  | NUM | MELT DESCRIPTION |  COEFF   |  VALUE
-------+-----+------------------+----------+---------
 Group |  1  | -CH3             |   -5.10  |   -5.10
 Group |  5  | CH (aromatic)    |    8.13  |   40.65
 Group |  1  | -C (aromatic)    |   37.02  |   37.02
   *   |     | Equation Constant|          |  122.50
============+==================+==========+=========
   RESULT    |  MELTING POINT in deg Kelvin |  195.07
             |  MELTING POINT in deg C      |  -78.09
-----------------------------------------------------
```

Notes

KOWWIN to Estimate
Octanol-Water Partition Coefficient (*KOW*)

What Is *KOW*?

KOW indicates whether a chemical predominantly will be found in water (is *hydrophilic*) or in fatty tissue of animals or other organic materials (is *lipophilic*) in an aquatic environment.

Important Note

KOW is often reported as a **log** due to the extremely wide range of measured *KOW* values.

Why Use the KOWWIN Model?

I need to know where the chemical will go in the stream - **Partitioning, Toxicity,** and *Bioconcentration.*

Partition-ing, Toxicity, Biocon-centra-tion

What Does the KOWWIN Model Do?

KOWWIN estimates a chemical's octanol-water partition coefficient (*KOW*).

Why Is *KOW* Important?

Lipophilic chemicals can *bioaccumulate* in fatty tissue of fish and *bioconcentrate* in animals (including humans) that consume the fish.

Chemicals with a Log *KOW* >5-6 can bioconcentrate significantly.

Relationship Between Log *KOW* and *BCF*

Log KOW

BCF

BCF

12
10
8
6
4
2
0

As log *KOW* increases the solubility in lipids increases. This means an increase in the potential to bioconcentrate in aquatic organisms. This relationship begins to change around log *KOW* of 6.

For chemicals with log *KOW* exceeding 6 the potential to bioconcentrate begins to drop approaching 0 at log *KOW* of 12.

KOWWIN to Estimate
Octanol-Water Partition Coefficient (*KOW*)

What You Need to Use KOWWIN

✓ CAS number or chemical structure in SMILES

Examples of *KOW* Values

CAS Number		Chemical	log *KOW*
lipophilic	60571	Dieldrin	5.2
	1912249	Atrazine	2.6
	58052	Caffeine	1.6
	75092	Dichloromethane	1.3
	50000	Formaldehyde	0.4
hydrophilic	67641	Acetone	-0.2

Inputs

✓ *CAS number* or chemical structure in SMILES notation

Important Note

A log KOW of 0 indicates an equal affinity for lipids and for water.

Outputs

✓ Log *KOW*

✓ Molecular weight and formula

✓ Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Saving Output

Output files can be saved as a ".dat" file or copied through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard.

Sample Output from the KOWWIN Model

INPUTS:

CAS Number = 60571 (dieldrin)

RESULTS:

```
                  Log Kow(version 1.66 estimate): 5.45


Experimental Database Structure Match:
  Name     :  Dieldrin
  CAS Num  :  000060-57-1
  Exp Log P:  5.40
  Exp Ref  :  DeBruijn,J et al. (1989)

Experimental Database Structure Match:
  Name     :  Endrin
  CAS Num  :  000072-20-8
  Exp Log P:  5.20
  Exp Ref  :  DeBruijn,J et al. (1989)


SMILES : CLC4=C(CL)C5(CL)C3C1CC(C2OC12)C3C4(CL)C5(CL)CL
CHEM   : Dieldrin
MOL FOR: C12 H8 CL6 O1
MOL WT : 380.91
```

TYPE	NUM	LOGKOW FRAGMENT DESCRIPTION	COEFF	VALUE
Frag	1	-CH2- [aliphatic carbon]	0.4911	0.4911
Frag	6	-CH [aliphatic carbon]	0.3614	2.1684
Frag	1	C [aliphatic carbon - No H, not tert]	0.9723	0.9723
Frag	2	=CH- or =C< [olefinc carbon]	0.3836	0.7672
Frag	1	-O- [oxygen, aliphatic attach]	-1.2566	-1.2566
Frag	4	-CL [chlorine, aliphatic attach]	0.3102	1.2408
Frag	2	-CL [chlorine, olefinic attach]	0.4923	0.9846
Frag	2	-tert Carbon [3 or more carbon attach]	0.2676	0.5352
Factor	2	Fused aliphatic ring unit correction	-0.3421	-0.6842
Const		Equation Constant		0.2290

```
                                             Log Kow   =   5.4478
```

Notes

WSKOW to Estimate Water Solubility

What Is Water Solubility?

Water solubility is the degree to which a compound will dissolve in water. It is reported as the amount of the chemical (in milligrams) that will dissolve in 1 liter of water (*mg/L*).

What Does the WSKOW Model Do?
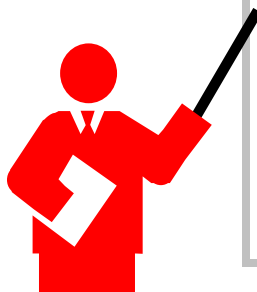
WSKOW uses the log *KOW* to estimate the compound's water solubility at 25ºC.

Why Use the WSKOW Model?

I need to know if the compound will dissolve in surface water - **Solubility.**

Solubility in Water
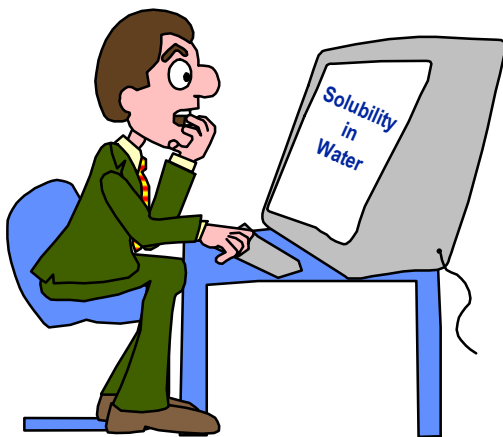
Why Is Knowing Solubility (S) Important?

Chemicals with low S will have low concentration in aqueous media. Chemicals with high S:

✓ Are more likely to be transported along with the water during storm events or through the water table; and

✓ Have low log *KOW* values, and are more likely to be absorbed through GI tract, or lungs. The exception is the case of dispersible molecules like surfactants, and detergents, which can have high predicted log KOWs and can be absorbed through the lung.

Solubility Classification (*mg/L* or ppm):

Very soluble	> 10,000
Soluble	> 1,000 - 10,000
Moderately sol.	> 100 - 1,000
Slightly soluble	> 0.1 - 100
Insoluble	< 0.1

WSKOW to Estimate Water Solubility

What You Need to Use WSKOW

✓ *CAS number* or chemical structure in SMILES

Examples of Water Solubility Values

CAS Number	Chemical	Water Sol. (*mg/L*)
67561	Methanol	1.00E+06
67641	Acetone	2.20E+05
50000	Formaldehyde	5.74E+04
1912249	Atrazine	2.14E+02
60571	Dieldrin	1.46E-01

Important Note

WSKOW is not appropriate for surfactants, which are dispersible.

Inputs

✓ *CAS number* or chemical structure in SMILES notation

Outputs

✓ Molecular weight and formula

✓ Water solubility at 25ºC (milligrams per liter)

✓ Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Saving Output

Output files can be saved as a ".dat" file or copied through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard.

Sample Output from the WSKOW Model

INPUTS:

CAS Number = 1912249 (atrazine)

RESULTS:

```
                  Water Sol: 214.1 mg/L


SMILES : n(c(nc(n1)NC(C)C)NCC)c1CL
CHEM   : Atrazine
MOL FOR: C8 H14 CL1 N5
MOL WT : 215.69
------------------------- WSKOW v1.37 Results --------------
Log Kow  (estimated)  :  2.82
Log Kow (experimental):  2.61
    Cas No: 001912-24-9
    Name  : Atrazine
    Refer : Hansch,C et al. (1995)
Log Kow used by Water solubility estimates:  2.61

Equation Used to Make Water Sol estimate:
   Log S (mol/L) = 0.796 - 0.854 log Kow - 0.00728 MW + Correction
      (used when Melting Point NOT available)

    Correction(s):         Value
    --------------------   -----
     No Applicable Correction Factors

   Log Water Solubility  (in moles/L) :    -3.003
   Water Solubility at 25 deg C (mg/L):   214.1
```

Notes

PCKOCWIN to Estimate
Organic Carbon Adsorption Coefficient (*KOC*)

What Is *KOC*?

KOC is the ratio of amount of chemical adsorbed per unit mass of organic carbon (the "OC") in soils, sediments, or sludge to the concentration of the chemical in the solution at equilibrium.

KOC indicates whether a chemical is likely to be be found in water or the organic carbon portion of soils or sediments.

What Does the PCKOCWIN Model Do?

PCKOCWIN estimates a chemical's soil sorption coefficient (*KOC*).

Why Use the PCKOCWIN Model?

I need to know where the chemical will go in the stream - **Partitioning.**

Parti-tioning

Important Note

Like KOW, *KOC* is also often reported as a **log** due to the extremely wide range of measured *KOC* values.

Why Is *KOC* Important?

KOC value provides an indication of whether or not a chemical will migrate with ground water.

High *KOC* indicates the chemical is likely to sorb to soils, sediments, or sludge and is less likely to migrate to ground water or to surface waters.

Low *KOC* indicates chemical is <u>not</u> likely to sorb to soils, sediments, or sludge, thus is more is likely to migrate to water.

PCKOCWIN to Estimate
Organic Carbon Adsorption Coefficient

What You Need to Use PCKOCWIN

✓ *CAS number* or chemical structure in SMILES

Examples of *KOC* Values

CAS Number	Chemical	Log *KOC*
60571	Dieldrin	4.025
1912249	Atrazine	2.362
75092	Dichloromethane	1.376
106898	Epichlorohydrin	0.652
67641	Acetone	0.297
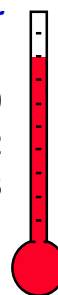
Sorption Values (log *KOC*)

Very strong	≥ 4.5
Strong	3.5 - 4.4
Moderate	2.5 - 3.4
Low	1.5 - 2.4
Negligible	< 1.5

Inputs

✓ *CAS number* or chemical structure in SMILES notation

Log *KOC* and Removal Rates

When Log *KOC* $\geq$4.5 chemical will be removed by sorption to sludge in wastewater treatment plants.

Outputs

✓ Estimated *KOC*

✓ Molecular weight and formula

✓ Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Saving Output

Output files can be saved as a ".dat" file or copied through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard.

Sample Output from the PCKOCWIN Model

INPUTS:

CAS Number = 98-86-2 (Acetophenone)

RESULTS:

```
                        Koc (estimated): 46.2



SMILES : O=C(c(cccc1)c1)C
CHEM   : Ethanone, 1-phenyl-
MOL FOR: C8 H8 O1
MOL WT : 120.15
----------------------- PCKOCWIN v1.66 Results -----------------------

        First Order Molecular Connectivity Index  ........... :   4.305
        Non-Corrected Log Koc  ............................. :   2.9123
        Fragment Correction(s):
                1    Ketone  (-C-CO-C-)  ................. : -1.2477
        Corrected Log Koc  ................................. :   1.6646

                    Estimated Koc:   46.2
```

Notes

HENRYWIN to Estimate
Henry's Law Constant

What Is Henry's Law Constant?

Henry's Law constant (HLC) is the ratio of a chemical's vapor pressure to its water solubility. HLC gives a relative measure of the volatility of a compound from water by measuring the extent to which a compound will partition between water and the air.

What Does the HENRYWIN Model Do?

HENRYWIN estimates the Henry's Law Constant (HLC) of an organic compound by two different methods. It also can estimate the HLC of an unknown compound based on the HLC of a known compound.

Why Use the HENRYWIN Model?

I need to know if the compound will volatilize from water or remain in the water.

HLC
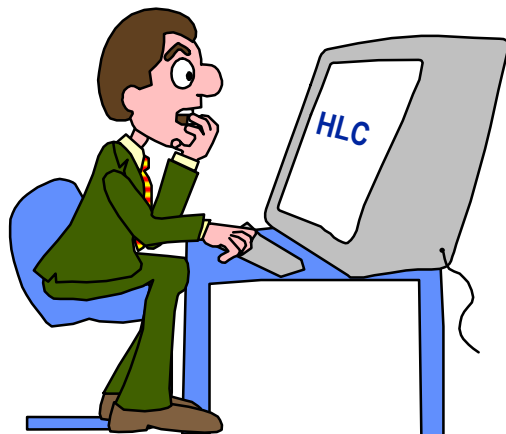
Why Is Knowing Henry's Law Constant Important?

Knowing the HLC helps the risk assessor predict the fate of the chemical once it is released to surface water.

✓ High HLC indicates chemical is likely to volatilize from solution and partition in air.

✓ Low HLC indicates chemical is not likely to volatilize and will remain in surface water.

HENRYWIN to Estimate
Henry's Law Constant

What You Need to Use HENRYWIN

✓ *CAS number* or chemical structure in SMILES

Examples of HLC Values

CAS Number	Chemical	HLC (atm-m^3/mole)
75092	Dichloromethane	3.0E-03
50000	Formaldehyde	6.1E-05
67641	Acetone	4.0E-05
67561	Methanol	4.4E-06
60571	Dieldrin	5.4E-07

Volatility Potential:

Very volatile	$\geq 10^{-1}$
Volatile	$10^{-1} - 10^{-3}$
Moderately volatile	$10^{-3} - 10^{-5}$
Slightly volatile	$10^{-5} - 10^{-7}$
Nonvolatile	$< 10^{-7}$

Inputs

✓ *CAS number* or chemical structure in SMILES notation

Outputs

✓ Molecular weight and formula

✓ Henry's Law Constant estimated by bond contribution method and by group contribution method (best used for pesticides)

✓ Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Saving Output

Output files can be saved as a ".dat" file or copied through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard.

Sample Output from the HENRYWIN Model

INPUTS:

CAS Number = 67561 (methanol)

RESULTS:

Bond Est	:	4.27E-006 atm-m3/mole
Group Est	:	3.62E-006 atm-m3/mole

> Two methods are used to estimate HLC. The group contribution method is best used for pesticides.

SMILES	:	OC
CHEM	:	Methanol
MOL FOR	:	C1 H4 O1
MOL WT	:	32.04

CLASS	|	BOND CONTRIBUTION DESCRIPTION	|COMMENT|	VALUE
HYDROGEN	| 3	Hydrogen to Carbon (aliphatic) bonds	| |	-0.3590
HYDROGEN	| 1	Hydrogen to Oxygen bonds	| |	3.2318
FRAGMENT	| 1	C-O	| |	1.0855
FACTOR	| *	Non-cyclic alkyl or olefinic alcohol	| |	-0.2000

RESULT	|	BOND ESTIMATION METHOD for LWAPC VALUE	| TOTAL |	3.758

HENRY'S LAW CONTSTANT at 25 deg C   =   4.27E-006 atm-m3/mole
                                     =   1.48E-004 unitless

	|	GROUP CONTRIBUTION DESCRIPTION	|COMMENT|	VALUE
	| 1	CH3 (X)	| |	-0.62
	| 1	O-H (C)	| |	4.45

RESULT	| GROUP ESTIMATION METHOD for LOG GAMMA VALUE	| TOTAL |	3.83

HENRY'S LAW CONTSTANT at 25 deg C   =   3.62E-006 atm-m3/mole
                                     =   1.48E-004 unitless

Notes

BCFWIN to Estimate *Bioconcentration* Factor

What Is *BCF*?

A *bioconcentration* factor (*BCF*) is the ratio (in L/kg) of a chemical's concentration in the tissue of an aquatic organism to its concentration in the ambient water.

Why Is *BCF* Important?

BCF indicates potential for a chemical to bioaccumulate in lipids (fatty tissue) of aquatic organisms, and to bioconcentrate as it moves up the food web.

Why Use a *BCF* Model?

I need to know if the chemical will bioaccumulate in aquatic life and move up the food chain.

What You Need to Use BCFWIN

✓ *CAS number* or chemical structure in SMILES

Relationship Between Log *KOW* and *BCF*

Log KOW

12
10
8
6
4
2
0

As log *KOW* increases the solubility in lipids increases. This means an increase in the potential to bioconcentrate in aquatic organisms. This relationship begins to change around log *KOW* of 6.
For chemicals with log *KOW* exceeding 6 the potential to bioconcentrate begins to drop approaching 0 at log *KOW* of 12.
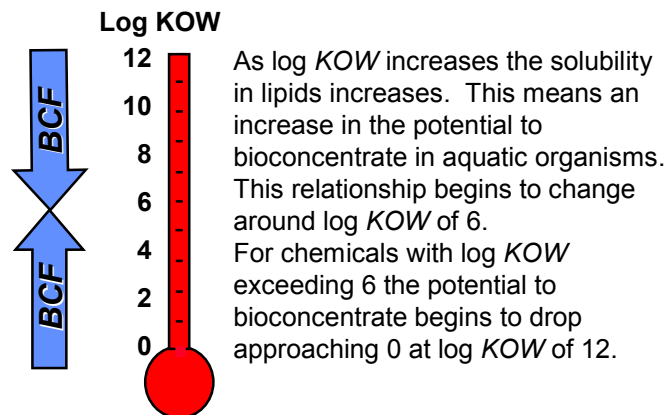
Bioconcentration Potential

High	≥1,000
Moderate	250 - 1,000
Low	<250

BCFWIN to Estimate *Bioconcentration* Factor

Examples of *BCF* Values

CAS Number	Chemical	Log *BCF*
8001352	Toxaphene	4.5
12789036	Chlordane	4.8
60571	Dieldrin	3.7
108703	1,3,5-Trichlorobenzene	2.7

Inputs

✓ *CAS number* or chemical structure in SMILES

Outputs

✓ Estimated Log *BCF*

✓ Estimated Log KOW

✓ Molecular weight and formula

Saving Output

Output files can be saved as a ".dat" file or copied through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard.

INPUTS:

CAS Number = 8001352 (toxaphene)

RESULTS:

```
        Log BCF (v2.14 estimate): 3.75


SMILES : CLC(C(CL)C1C2)C(C2(CL)CL)(C1(C(CL)CL)CCL)CCL
CHEM   : Toxaphene
MOL FOR: C10 H10 CL8
MOL WT : 413.82
----------------- Bcfwin v2.14 --------------------
Log Kow  (estimated)  :  6.79
Log Kow (experimental):  5.78
Log Kow used by BCF estimates:  5.78


Equation Used to Make BCF estimate:
   Log BCF = 0.77 log Kow - 0.70 + Correction


     Correction(s):                    Value
       No Applicable Correction Factors


   Estimated Log BCF =  3.751  (BCF = 5631)
```

Models to Estimate
Chemical Fate in the Environment

Following are brief fact sheets providing information on the models OPPT uses to estimate the fate of a chemical once it is released to the environment. Information provided on each model includes:

- ✓ What fate property does the model estimate?

- ✓ What is significant about the fate property to exposure assessment?

- ✓ Why is knowing the fate property important?

- ✓ Why would I want to use the model?

- ✓ What do I need to run the model?

- ✓ What are the inputs and outputs for the model?

FATE MODELS

AOPWIN

BIOWIN

HYDROWIN

STPWIN
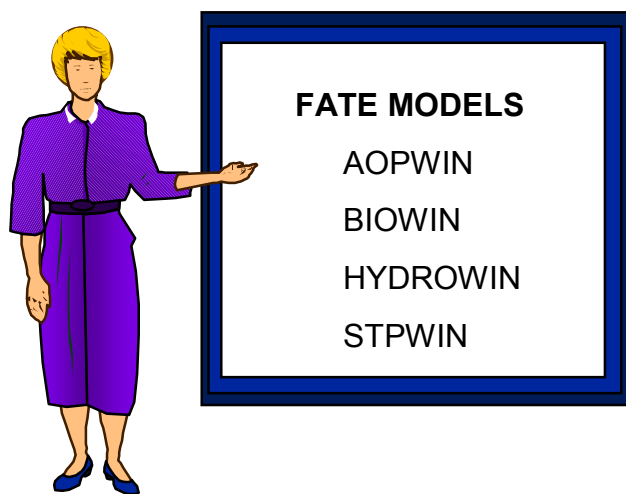
Notes

AOPWIN to Estimate
Atmospheric Oxidation Potential

What Is AOP?

The Atmospheric Oxidation Program (AOP) estimates *rate constants* and *half-lives* of atmospheric reactions of organic compounds released to the air with hydroxyl radicals (-OH) and with ozone in the atmosphere.

What Does the AOPWIN Model Do?

AOPWIN estimates the rate at which certain organic compounds will be destroyed by reactions with compounds in the atmosphere.

Why Use the AOPWIN Model?

I need to know how long it will take for an organic compound to be destroyed by reactions in the air - **Atmospheric Oxidation Potential**.

Atmospheric Oxidation Potential

Why Is Atmospheric Oxidation Important?

The rate at which an organic compound will be oxidized (destroyed) indicates the length of time the compound may reside in the atmosphere. This also is known as the chemical's atmospheric residence time.

Important Note

If a chemical has a high AOP rate there still is a potential for inhalation exposure if the travel time from source to receptor is greater than the time for complete oxidation of the compound.

AOPWIN to Estimate
Atmospheric Oxidation Potential

What You Need to Use AOPWIN

✓ *CAS number* or chemical structure in SMILES

Examples of AOP Values

CAS Number	Chemical	AOP 1/2 Life (days)
75092	Dichloromethane	79.3
67641	Acetone	52.4
67561	Methanol	17.4
60571	Dieldrin	1.2
1912249	Atrazine	0.4
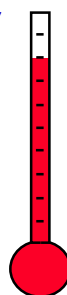
AOP *Half-life* Value Classifications

Rapid	$\leq$ 2 hrs
Moderate	2 hrs - $\leq$ 1 day
Slow	> 1 day - $\leq$ 10 days
Negligible	> 10 days

Half-life of >2 days indicates the chemical will be persistent in air.

Inputs

✓ *CAS number* or chemical structure in SMILES notation

Outputs

✓ Molecular weight and formula

✓ Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

✓ Hydroxyl radical (-OH) rate constant and *half-life*

✓ Ozone reaction constant and *half-life* (for olefins and acetylenes only)

Saving Output

Output files can be saved as a ".dat" file or copied through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard.

Sample Output from the AOPWIN Model

INPUTS:

CAS Number = 1912249 (atrazine)

RESULTS:

```
SMILES      :   n(c(nc(n1)NC(C)C)NCC)c1CL
CHEM        :   Atrazine
MOL FOR     :   C8 H14 CL1 N5
MOL WT      :   215.69
```
---------------------------------SUMMARY : HYDROXYL RADICALS---------------------------------

Hydrogen Abstraction	=	24.2300 E-12 cm3/molecule-sec
Reaction with N, S, and -OH	=	0.0000 E-12 cm3/molecule-sec
Addition to Triple Bonds	=	0.0000 E-12 cm3/molecule-sec
Addition to Olefinic Bonds	=	0.0000 E-12 cm3/molecule-sec
**Addition to Aromatic Rings	=	0.1176 E-12 cm3/molecule-sec
Addition to Fused Rings	=	0.0000 E-12 cm3/molecule-sec
OVERALL OH	=	27.3476 E-12 cm3/molecule-sec
HALF-LIFE	=	0.391 Days (12-hr day; 1.5E6 OH/cm3)
HALF-LIFE	=	4.693 Hrs

. . . . * * Designates Estimation(s) Using ASSUMED Value(s) . . . .

--------------------------SUMMARY (AOP v1.90): OZONE REACTION--------------------------

* * * * * * *   NO OZONE REACTION ESTIMATION   * * * * * * * *
(ONLY Olefins and Acetylenes are Estimated)

Experimental Database : NO Structure Matches

> Reactions with ozone are estimated only for olefins and acetylenes.

Notes

BIOWIN to Estimate Biodegradation

What Does the BIOWIN Model Do?

BIOWIN estimates the time required for a compound to biodegrade in a stream.

What Is Biodegradation?

Biodegradation is the transformation of a compound by biota, typically microorganisms, in the environment. Primary biodegradation is a change in molecular structure, and ultimate biodegradation is the destruction of the molecule.

Why Is Biodegradation Important?

Knowing the time required for a chemical to be broken down will help the risk assessor estimate the likely concentration of the chemical at various locations and times after release to a stream.

Chemicals with very long biodegradation times may be highly persistent in the environment IF they are not subject to destruction by other processes such as photolysis, hydrolysis, etc.

Why Use the BIOWIN Model?

I want to know the time needed for the chemical to degrade once it is released to the stream - **Biodegradation.**

Biodeg-radation

BIOWIN Uses Linear and Non-linear Models

Two models are used by BIOWIN, a linear and a non-linear regression model. The models are based on regressions against 36 preselected chemical substructures plus molecular weight for experimental biodegradation data for 295 chemicals. The models correctly classified 90% of the chemicals in their training set as rapidly or not rapidly *biodegradable*. Results were slightly better for the nonlinear model.

BIOWIN to Estimate Biodegradation

What You Need to Use BIOWIN

✓ *CAS number* or chemical structure in SMILES
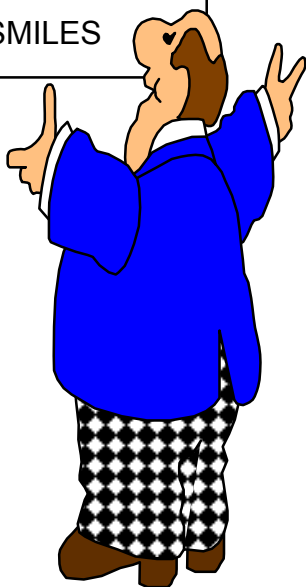
Examples of Biodegradation Rates

CAS Number	Chemical	Ultimate Biodeg. (weeks)
60571	Dieldrin	recalcitrant
1912249	Atrazine	months
75092	Dichloromethane	weeks-months
67641	Acetone	weeks
67561	Methanol	days-weeks
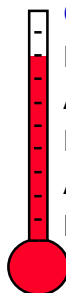
Biodegradation Rates

Rapid	$\geq$ 60% in	$\leq$ 7 days
Moderate	$\geq$ 30% in	$\leq$ 28 days
Slow	< 30% in	$\leq$ 28 days
Very slow	< 30% in	> 28 days

Inputs

✓ *CAS number* or chemical structure in SMILES notation

Saving Output

Output files can be saved as a ".dat" file or copied through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard.

Outputs

✓ Molecular weight and formula

✓ Predicted primary and ultimate biodegradation in hours, days, weeks, or months; also predicted, via separate but by linked model, the probability of fast biodegradation using two different methods

✓ Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Sample Output from the BIOWIN Model

```
INPUTS:              CAS Number = 67561 (methanol)
RESULTS:
SMILES  :  OC
CHEM    :  Methanol
MOL FOR :  C1 H4 O1
MOL WT  :  32.04
------------------------- BIOWIN v4.00 Results -------------
    Linear Model Prediction  :  Biodegrades Fast
    Non-Linear Model Prediction:  Biodegrades Fast
    Ultimate Biodegradation Timeframe:  Days-Weeks
    Primary  Biodegradation Timeframe:  Days
    MITI Linear Model Prediction  :  Readily Degradable
    MITI Non-Linear Model Prediction:  Readily Degradable
------+-----+---------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+---------------------------------------+---------+---------
 Frag |  1  | Aliphatic alcohol  [-OH]              | 0.1587  | 0.1587
 MolWt|  *  | Molecular Weight Parameter            |         | -0.0153
 Const|  *  | Equation Constant                     |         | 0.7475
===========+=======================================+=========+=========
   RESULT   |     LINEAR BIODEGRADATION PROBABILITY  |         | 0.8910
===========+=======================================+=========+=========
------+-----+---------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+---------------------------------------+---------+---------
 Frag |  1  | Aliphatic alcohol  [-OH]              | 1.1178  | 1.1178
 MolWt|  *  | Molecular Weight Parameter            |         | -0.4550
===========+=======================================+=========+=========
   RESULT   |   NON-LINEAR BIODEGRADATION PROBABILITY |        | 0.9752
===========+=======================================+=========+=========
 A Probability Greater Than or Equal to 0.5 indicates --> Biodegrades Fast
 A Probability Less Than 0.5 indicates --> Does NOT Biodegrade Fast
------+-----+---------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+---------------------------------------+---------+---------
 Frag |  1  | Aliphatic alcohol  [-OH]              | 0.1600  | 0.1600
 MolWt|  *  | Molecular Weight Parameter            |         | -0.0708
 Const|  *  | Equation Constant                     |         | 3.1992
===========+=======================================+=========+=========
   RESULT   |   SURVEY MODEL - ULTIMATE BIODEGRADATION |       | 3.2883
===========+=======================================+=========+=========
------+-----+---------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+---------------------------------------+---------+---------
 Frag |  1  | Aliphatic alcohol  [-OH]              | 0.1294  | 0.1294
 MolWt|  *  | Molecular Weight Parameter            |         | -0.0462
 Const|  *  | Equation Constant                     |         | 3.8477
===========+=======================================+=========+=========
   RESULT   |   SURVEY MODEL - PRIMARY BIODEGRADATION |        | 3.9310
===========+=======================================+=========+=========
 Result Classification:   5.00 -> hours    4.00 -> days    3.00 -> weeks
  (Primary & Ultimate)    2.00 -> months   1.00 -> longer
------+-----+---------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+---------------------------------------+---------+---------
 Frag |  1  | Aliphatic alcohol  [-OH]              | 0.1611  | 0.1611
 Frag |  1  | Methyl  [-CH3]                        | 0.0004  | 0.0004
 MolWt|  *  | Molecular Weight Parameter            |         | -0.0953
 Const|  *  | Equation Constant                     |         | 0.7121
===========+=======================================+=========+=========
   RESULT   |   MITI LINEAR BIODEGRADATION PROBABILITY |       | 0.7784
===========+=======================================+=========+=========
------+-----+---------------------------------------+---------+---------
 TYPE | NUM |       BIOWIN FRAGMENT DESCRIPTION      |  COEFF  |  VALUE
------+-----+---------------------------------------+---------+---------
 Frag |  1  | Aliphatic alcohol  [-OH]              | 1.0041  | 1.0041
 Frag |  1  | Methyl  [-CH3]                        | 0.0194  | 0.0194
 MolWt|  *  | Molecular Weight Parameter            |         | -0.9250
===========+=======================================+=========+=========
   RESULT   | MITI NON-LINEAR BIODEGRADATION PROBABILITY |     | 0.9324
===========+=======================================+=========+=========
 A Probability Greater Than or Equal to 0.5 indicates --> Readily Degradable
 A Probability Less Than 0.5 indicates --> NOT Readily Degradable
```

This chemical biodegrades completely in days to weeks.

Notes

HYDROWIN to Estimate Hydrolysis

What Is Aquatic Hydrolysis?

Once a chemical enters a surface water body, it may react with water in a manner in which the water molecule, or the hydroxide ion, displaces an atom or group of atoms in the chemical.

What Does the HYDROWIN Model Do?

HYDROWIN estimates acid- and base-catalyzed rate constants for certain *chemical classes* (esters, carbamates, epoxides, halomethanes, and certain alkyl halides). The rate constants are used to calculate hydrolysis half-lives at selected pHs.

Why Use the HYDROWIN Model?

I need to know if the chemical will react with water in the stream - **Hydrolysis.**

Hydrolysis

Why Is Hydrolysis Important?

The rate at which a compound reacts with (and is broken down by) water helps a risk assessor estimate the concentration of the compound after it is released to surface water. Understanding hydrolysis is important in determining the fate of the chemical in water.

HYDROWIN to Estimate Hydrolysis

What You Need to Use HYDROWIN

✓ *CAS number* or chemical structure in SMILES

Examples of Hydrolysis Rates

CAS Number	Chemical	Hydrolysis 1/2 Life (yrs)
51796	Carbamic acid, ethyl ester	3326.534
110383	Ethyl decanonate	7.7

Inputs

✓ *CAS number* or chemical structure in SMILES notation

Outputs

✓ Molecular weight and formula

✓ Estimated hydrolysis at 25ºC

✓ *Half-life* at pHs 8 and 7

✓ Chemical structure can be printed or saved as either MDL ISIS SKC file or MDL MOL file

Saving Output

Output files can be saved as a ".dat" file or copied through the Windows Clipboard. Structures can be saved as an ISIS ".skc" file or through the Windows Clipboard.

Sample Output from the HYDROWIN Model

INPUTS:

CAS Number = 110-38-3 (Ethyl decanonate)

RESULTS:


```
SMILES : O=C(OCC)CCCCCCCCC
CHEM   : Decanoic acid, ethyl ester
MOL FOR: C12 H24 O2
MOL WT : 200.32
--------------------- HYDROWIN v1.67 Results ----------------------

NOTE: Fragment(s) on this compound are NOT available from the
fragment
    library. Substitute(s) have been used!!!  Substitute R1, R2, R3,
    or R4 fragments are marked with double asterisks "**".

ESTER:  R1-C(=O)-O-R2              ** R1: n-Octyl-
                                      R2: -CH2-CH3
 Kb hydrolysis at atom #  2:  2.848E-002  L/mol-sec


 Total Kb for pH > 8 at 25 deg C :  2.848E-002  L/mol-sec
 Kb Half-Life at pH 8:     281.632 days
 Kb Half-Life at pH 7:       7.711  years
```

Notes

STPWIN to Estimate
Percent Removal in Wastewater Treatment

What Are "STPs" and "POTWs"?

STP is "Sewage Treatment Plant," and POTW is "Publicly Owned Treatment Works." Both are names for utilities that treat waste water and usually discharge the treated water to nearby surface water bodies.

What Does the STPWIN Model Do?

STP predicts the percent of a compound that will be removed from the waste water in wastewater treatment.

Why Use the STPWIN Model?

I need to know how much of the chemical will be removed from the waste water during treatment in the POTW.

Percent Destroyed in the POTW

Why Is Knowing the Percent Destroyed in a POTW Important?

Knowing how much of the chemical will be removed from waste water during wastewater treatment enables the risk assessor to predict how much of the chemical may be discharged by the POTW to surface water and potentially affect aquatic life.

STPWIN to Estimate
Percent Removal in Wastewater Treatment

Examples of Removal Rates

CAS Number	Chemical	Removal in STP (%)
60571	Dieldrin	83.11
75092	Dichloromethane	55.11
50000	Formaldehyde	67.3
67641	Acetone	73.06
108952	Phenol	97.47

What You Need to Use STPWIN

✓ *CAS number* or chemical structure in SMILES

Outputs

✓ Percent removal in wastewater treatment

✓ Overall chemical mass balance

Sample Output from the STPWIN Model

```
INPUTS:                    SMILES : c1ccccc1
```
```
RESULTS:
SMILES :   c1ccccc1
CHEM   :   Chemical B
MOL FOR:   C6 H6
MOL WT :   78.11
-------------------------- EPI SUMMARY (v3.01) -----------------------
 Physical Property Inputs:
    Water Solubility (mg/L):   1800
    Vapor Pressure (mm Hg) :    95.3
    Henry LC (atm-m3/mole) :  ------
    Log Kow (octanol-water):  ------
    Boiling Point (deg C)  :  ------
    Melting Point (deg C)  :  ------

STP Fugacity Model:  Predicted Fate in a Wastewater Treatment Facility
=====================================================================
PROPERTIES OF: Chemical B
-------------
Molecular weight (g/mol)      78.11
Aqueous solubility (mg/l)     1800
Vapour pressure (Pa)          12705.6
              (atm)           0.125395
              (mm Hg)         95.3
Henry 's law constant (Atm-m3/mol)        0.00555
Air-water partition coefficient           0.226978
Octanol-water partition coefficient (Kow)     134.896
Log Kow                                   2.13
Biomass to water partition coefficient        27.7793
Temperature [deg C]                       25
Biodeg rate constants (h^-1),half life in biomass (h) and in 2000 mg/L MLSS (h):
  -Primary tank       0.00      526.34                 10000.00
  -Aeration tank      0.00      526.34                 10000.00
  -Settling tank      0.00      526.34                 10000.00


 STP Overall Chemical Mass Balance:
 --------------------------------
                            g/h          mol/h        percent
Influent                 1.00E+001     1.3E-001       100.00

Primary sludge           5.63E-002     7.2E-004         0.56
Waste sludge             5.46E-002     7.0E-004         0.55
Primary volatilization   1.25E-001     1.6E-003         1.25
Settling volatilization  1.10E-001     1.4E-003         1.10
Aeration off gas         6.54E+000     8.4E-002        65.43

Primary biodegradation   1.82E-003     2.3E-005         0.02
Settling biodegradation  1.76E-004     2.2E-006         0.00
Aeration biodegradation  2.35E-003     3.0E-005         0.02

Final water effluent     3.11E+000     4.0E-002        31.06

Total removal            6.89E+000     8.8E-002        68.94
Total biodegradation     4.35E-003     5.6E-005         0.04
```

Notes

Models to Estimate
Hazard to Humans and the Environment

Following are brief fact sheets providing information on the models OPPT uses to estimate *hazard* to humans and the environment from exposure to chemicals released to the environment. Information provided on each model includes:

- ✓ What *hazard* does the model estimate?

- ✓ What is significant about the *hazard* to exposure assessment?

- ✓ Why is knowing the *hazard* important?

- ✓ Why would I want to use the model?

- ✓ What do I need to run the model?

- ✓ What are the inputs and outputs for the model?

HAZARD **MODELS**

OncoLogic

ECOSAR
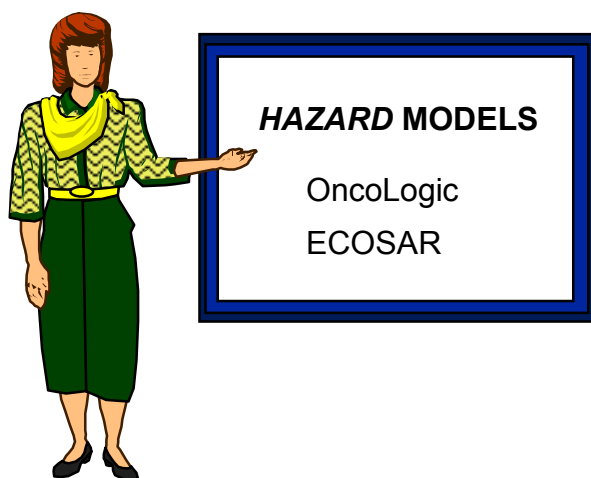
Notes

OncoLogic to Estimate Potential Carcinogenicity

What Does the Model Do?

OncoLogic estimates the potential *carcinogenicity* of a chemical.
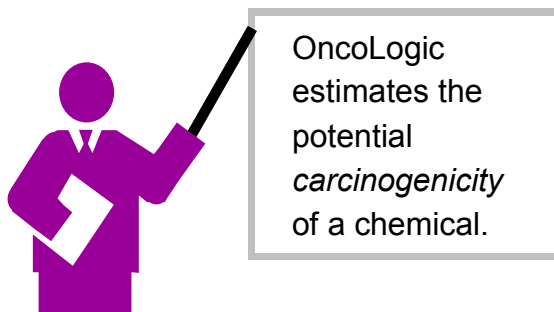
How Does the Model Work?

OncoLogic estimates the potential for a chemical to cause cancer in humans using the known *carcinogenicity* of chemicals with similar chemical structures, information on mechanisms of action, short-term predictive tests, epidemiological studies, and expert judgment.

Why is *Carcinogenicity* of a Chemical Important?

An understanding of the potential for the chemical to cause cancer helps the risk assessor estimate the impact of the release on the surrounding human population.

Why Use the OncoLogic Model?

I need to know the potential for the chemical to cause cancer in humans - **Carcinogenicity.**

I also need to know if I should do further testing of the chemical - *Bioassays.*
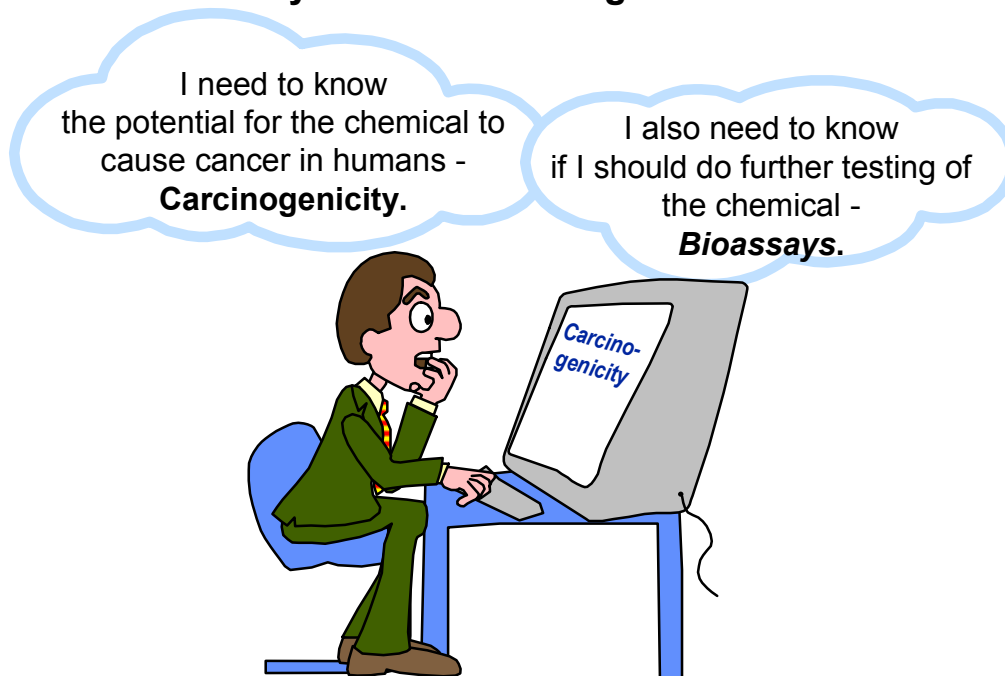
Carcino-genicity

OncoLogic to Estimate
Potential Carcinogenicity

Inputs

✓ Class of chemical (fiber, polymer, metal, or organic compound)

✓ Chemical structure

✓ Functional groups present

✓ Additional properties listed in Flow Diagrams for each module.

What You Need to Use OncoLogic

✓ Good understanding of organic chemistry
✓ *Chemical class* of the compound
✓ Certain physical and chemical properties of the compound

Important Note

OncoLogic has modules to estimate *carcinogenicity* of 4 types of compounds:

✔ Fibers   ✔ Metals

✔ Polymers   ✔ Organics

Outputs

✓ Summary of predicted concern level (high to low)

✓ Line of reasoning for estimation

OncoLogic Model
Flow Diagram

Select Option

Fibers*

Polymers*

Metals*

Organics*

Inputs: Chemical Information
Requested by Module
(See Following Flow Diagrams
for Specific Module Inputs)
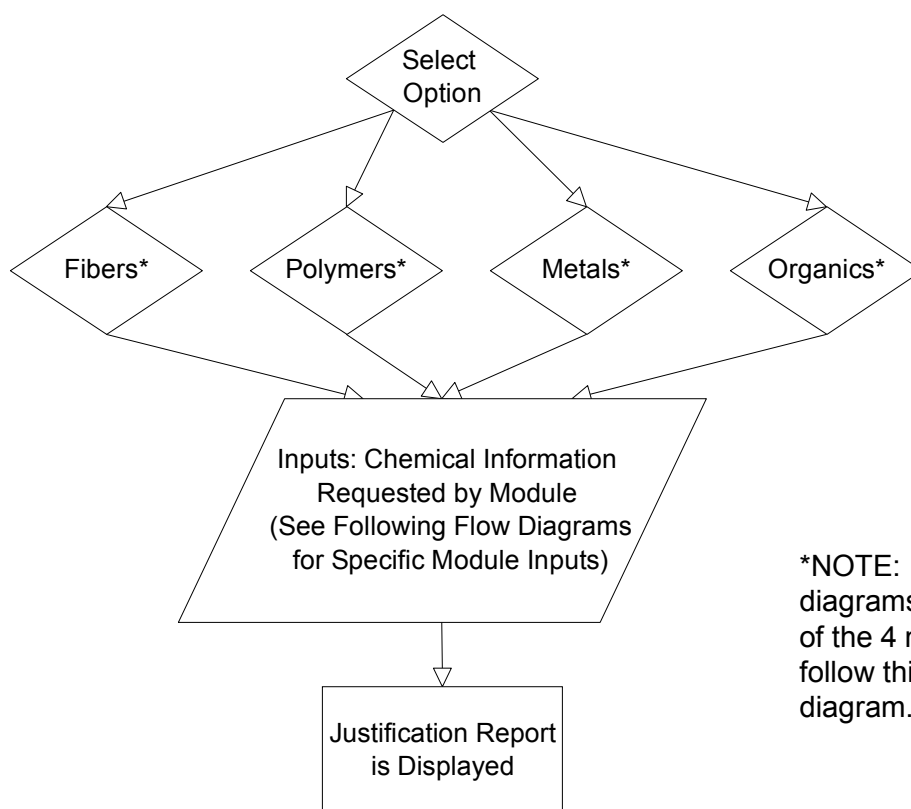
*NOTE: Flow
diagrams for each
of the 4 modules
follow this basic
diagram.

Justification Report
is Displayed

OncoLogic Model Flow Diagram - Fibers

```
              ╱─────────────────╲
             ╱  Enter:            ╲
            ╱  Chemical's Unique   ╲
            ╲  File Name*          ╱
             ╲───────────────────╱
                     │
                     ▽
  ┌──────────────┐  ╱─────────────────╲
  │ Evaluate in  │ ◁ Enter:            ╲
  │ another ONCO │ ╱ Chemical's Unique  ╲
  │ Module       │ ╲ Substance ID*      ╱
  └──────────────┘  ╲───────────────────╱
                          │
                          ▽
                 ╱─────────────────╲
                ╱  Enter:            ╲
               ╱  Water Solubility    ╲
               ╲  (Y/N/Unk)          ╱
                ╲───────────────────╱
                          │
                          ▽
```

Inputs Needed for Fibers Evaluation:

Water solubility (yes/no)

Diameter (microns)

Length (microns)

Additional Inputs Needed for Refining the Evaluation Are:

Presence of electrical charge

Properties[+]

    Flexibility

    Durability

    In vivo biodegradability

    Surface characteristics

    Splitting properties

Moieties[#]

    High molecular weight polymer

    Low molecular weight organic *moiety*

    Metals or metalloids

Manufacturing process

Use scenario

Enter: Diameter (microns)
Length (microns)
High Density Charge? (Y/N/Unk)
Additional Properties+ (if known)
Additional *Moieties*# (if known)

Enter: Manufacturing Process

Select: Standard Evaluation or Worst Case Scenario

Justification Report is Displayed

*NOTE: The chemical's file name and substance ID are unique names that the user enters. The chemical's file name is limited to 8 characters. The program will take up to 240 characters for the chemical's substance ID.

Sample Output from OncoLogic Fibers Justification Report

INPUTS:

Chemical file name	=	Fiber1	High density charge	=	Unk
Substance Id	=	Fiber1			

Additional properties:

Water soluble	=	No	Durability	✓	
Diameter	=	0.1 - 0.5 microns			
Moieties	=	none	Median(s)	=	0Manufacturing
process	=	Crystallization	Length	=	1 - 3 microns
Scenario evaluation	=	Standard	Aspect ratio	=	0

Justification Report is saved in ONCO dir. as ASCII file as "Chemical file name.JST"

RESULTS:

SUMMARY:

Code Number: Fiber1

Substance Id: Fiber1

The final level of this fiber-type substance is HIGH.

JUSTIFICATION:

STANDARD EVALUATION

The unifying concept of fiber carcinogenisis is the Stanton Hypothesis. This hypothesis states that the dimensions of a fiber are the major criteria for establishing the concern for its *carcinogenic* potential.

The STANDARD evaluation is the accepted method for determining the *carcinogenic* potential of a fiber. It is based on the median diameter and length. The distribution of dimensions is assumed to be uniform. When a range is entered, the program calculates the median as the average of the high and low values.

Since the diameter of the fiber is equal to or greater than 0.25 microns and less than 1.5 microns, and its aspect ratio is greater than 5 and not more than 32, the initial level of concern for *carcinogenic* potential of this fiber is MODERATE.

Naturally occurring fibers and synthetic fibers that are manufactured through a crystallization process are assumed to have strong electron donor/basic sites on their surface, since these conditions provide time for orderly build-up of surface structure. This increases the level of concern to HIGH-MODERATE.

The fiber exhibits the following property or properties: durability. These characteristics make minor modifications to the concern level and many are inter-related. Thus, regardless of the number of these characteristics the fiber exhibits, the final level of concern is increased by only one step to HIGH.

The final concern for this fiber-type substance is HIGH.

OncoLogic Model Flow Diagram - Polymers

Enter: Chemical's Unique File Name* and Substance ID *

↓

Answer Question on Covalently Linked Repeating Subunits

↓

Answer Question on Residual Monomers

↓

Answer Questions on Low Molecular Weight Species

↓

Answer Question on Metals/Metalloids

↓

Answer Question on Cross-linking

↓

Answer Question on Reactive Functional Groups (RFGs)

↓

Answer Question on Water Solubility*

↓

Answer Questions on Polyfunctionality (RFG equivalent weight, interjunction distance)

↓

Answer Question on Hyperplasitc Effects

↓

Answer Question on Ingestion

↓

Answer Question on Releasable Subunits

↓

Justification Report is Displayed

Inputs Needed for Polymers Evaluation:

Molecular weight

Water solubility and behavior in water

Polyfunctional behavior

Hyperplastic effects

Possible Ingestion

Information on chemical structure/properties, including presence of:

> Covalently-linked units
>
> Residual monomer
>
> Residual functional groups
>
> Low molecular weight species
>
> Metals or metalloids
>
> Cross-linkages
>
> Reactive functional groups
>
> Internal releasable subunits
>
> Terminal/pendant releasable subunits

* If water solubility is in ppm, convert to percent by dividing the number by 10,000. If water solubility is unknown, enter 0.

Sample Output from OncoLogic Polymers Justification Report

INPUTS:

Chemical file name	=	Polymer1
Substance Id	=	Polymer substance A
Molecular weight	=	1,100
Covalently linked units	=	Yes
Residual monomers >2%	=	No
Low MW species (<500) present	=	Yes
Polymer reactive functional groups (RFGs)	=	Yes
RFGs present	=	Oxygen
Oxygen RFG	=	Epoxide (unsubstituted)
Additional RFGs present	=	No
Metals/Metalloids present	=	No
Crosslinkages present	=	No
Polymer RFGs present	=	Yes
Identify Polymer RFG	=	Oxygen
Oxygen RFG	=	Epoxide (unsubstituted)
Additional RFGs present	=	No
Water solubility as percent weight	=	0.2
Polyfunctional	=	Yes
Functional groups equivalent. wt.	=	550
Interjunction distance	=	Yes
Hyperplastic effects	=	No
Absorption into soft tissue	=	Unknown
Ingestion possible	=	Yes
Internal release subunits	=	No
Terminal pendant subunits	=	No

Justification Report is saved in ONCO directory as ASCII file as "Chemical file name.JST"

RESULTS:

SUMMARY:

CODE NUMBER: polymer1

SUBSTANCE ID: polymer substance A

The final level of *carcinogenicity* concern for this polymer is LOW MODERATE.

Based on the reactive functional group Epoxide (unsubstituted), the level of concern for the low molecular weight species LOW MODERATE.

CAUTIONARY NOTES:
1. Plasticizers and other additives, if present, should be evaluated separately in the Organics Subsystem.

2. Counterions of polymers with ionic backbones should be evaluated separately.

Sample Output from OncoLogic Polymers Justification Report

Continued from previous page

JUSTIFICATION:

Because the substance consists of covalently linked repeating units and has a molecular weight greater than or equal to 1000, the substance is classified as a high molecular weight polymer.

Since the polymer contains less than 2% residual monomer(s), the *carcinogenicity* concern for any residual monomers is LOW.

The polymer contains low molecular weight species (>2% below 500), with a reactive-functional-group-bearing sidechain. The level of *carcinogenicity* concern for the low molecular weight species is based on the reactive functional group: Epoxide (unsubstituted).

The level of *carcinogenicity* concern for the low molecular weight species is LOW MODERATE.

The polymer is not cross-linked.

Since the percent water solubility is greater than or equal to 0.1%, the polymer is considered to be soluble in water.

The reactive functional group (RFG) which was used during the evaluation of the polymer is: Epoxide (unsubstituted).

This water soluble polymer is polyfunctional. Based on the expert-assigned inherent *carcinogenic* potential of the RFG(s) that you have entered and the entered information on the functional group equivalent weight of 550 daltons, which is low enough to cause concern, and the interjunction distance of less than ten atoms, which is within the favorable distance for potential cross-linking, the RFG which is retained for the evaluation of the polymer is Epoxide (unsubstituted).

Since this polymer has been demonstrated not to cause (or is not known to have caused) inflammatory and/or hyperplastic changes, *carcinogenicity* concerns arising from these pathophysiological changes can be eliminated.

The RFG which is contained in this polymer is known to be stable in solution or as an emulsion in water. The current level of *carcinogenicity* concern based on the RFG is retained.

The water soluble polymer has a molecular weight less than or equal to 5,000. The polymer contains reactive-functional-group-bearing sidechains but has not (or is not known to have) demonstrated an ability to be absorbed and to accumulate in soft tissue. Therefore, the level of *carcinogenicity* concern for this polymer is LOW MODERATE.

The final concern for this polymer is LOW MODERATE.

OncoLogic Model Flow Diagram - Metals

Enter: Chemical's Unique File Name* and Substance ID *

Is Chemical Radioactive, or Does it Contain Radioactive Metals/Metalloids?

Yes → Analysis ends here. Program does not evaluate radioactive compounds.

No

Anwer Questions on Metals/Metalloids Present:
Select: Metals Present
Is Metallized Dye Present
Enter Metal Classification
Enter Oxidation State

Answer Question on Water Solubility*

Answer Question on Crystalline Lattice

Enter Expected Routes of Exposure

Answer Question Organic Moiety

Justification Report is Displayed

Inputs Needed for Metals Evaluation:

Chemical structure

Radioactivity

Presence of metallized dye or pigment

Metal classification

Oxidation state

Water solubility

Crystalline lattice present?

Routes of exposure expected

Organic *moiety* under physiological conditions

* If water solubility is in ppm, convert to percent by dividing the number by 10,000. If water solubility is unknown, enter 0.

Sample Output from OncoLogic Metals
Justification Report

INPUTS:					
Chemical file name	=	Crystal	Oxidation state	=	Hexavalent
Substance Id	=	Crystal	Water solubility	=	Sparingly soluble
Radioactivity	=	No	Crystalline lattice	=	Yes
Metals present	=	Cr and Zr	Route of exposure	=	Inhalation
Metallized dye or pigment	=		No	Organic *moiety*	=
No		Metal classification	=		Inorganic or other

comp.
Justification Report is saved in ONCO directory as ASCII file as "Chemical file name.JST"

RESULTS:

Code Number: crystal
Substance Id: crystal

SUMMARY:

The final level of concern for this Cr-containing inorganic or organic compound, when the anticipated exposure is via the inhalation route, is HIGH.

JUSTIFICATION:

Since this substance contains more than one metal, Cr, Zr, the system has considered all metals present. The level of concern and the line of reasoning are based on the metal which provides the highest level of *carcinogenicity* concern. When more than one metal gives the same highest level of concern, the line of reasoning is given for only one of the metals.

In general, virtually all Cr-containing compounds are of some *carcinogenicity* concern unless they can be clearly shown to be not bioavailable. Exposure to these compounds by inhalation or injection is of greater concern than exposure by the oral or dermal route.

The *carcinogenic* potential of inorganic chromium compounds is affected by their oxidation state, crystallinity, and solubility, which affect the extent of compound uptake by cells. Hexavalent compounds are more easily taken up by cells than trivalent; and crystalline compounds are more easily taken up than amorphous compounds. Sparingly soluble and insoluble compounds are more likely than soluble compounds to be retained at the site of exposure, and thus have more of an opportunity to be taken up by the cells. Organic chromium compounds containing a Cr-C covalent bond are treated as inorganic compounds because the Cr-C covalent bond is expected to be easily hydrolyzed in aqueous solution.

Since the substance is a(an) inorganic or organic compound, and the oxidation state of chromium is hexavalent, and exposure to this sparingly soluble, crystalline substance is expected to be by the inhalation route, the level of *carcinogenicity* concern is HIGH.

The final level of concern for this Cr-containing inorganic or organic compound, when the anticipated exposure is via the inhalation route, is HIGH.

OncoLogic Model Flow Diagram - Organics

New or Previous Evaluation?

Enter: Chemical's Unique File Name*

Select: Organic Class

Enter: Chemical's Unique Substance ID *

Select: Aromatic Amine-related Compound

Answer Question on Amine-generating Groups

Select: Aryl Rings

Is Chemical (CAS No., name, structure) in Database?

Build Structure by Adding Groups Present: Rings, Heteroatoms, Intercyclic Linkages, Subunits

Justification Report is Displayed

Inputs Needed for Organics Evaluation:

Organic *chemical class*

CAS number/Chemical name (if listed)

Molecular structure, including presence of:

- Rings
- Functional groups
- Linkages
- Substituents

NOTE:
*The chemical's file name and substance ID are unique names that the user enters. The chemical's file name is limited to 8 characters. The program will take up to 240 characters for the chemical's substance ID.

Sample Output from OncoLogic Organics Justification Report

INPUTS:

Chemical file name = Amine1

Organic class = Aromatic amine

Substance Id = Aromatic amine#1

Aromatic-related compound class = None

Amine-generating group = Yes

Aryl rings selected:

   6-member rings = 1

   Heteroatoms = No

Answers are correct

Structure building:

Select:

   - Build

   - Add

   - Substituents

   - Alkoxy (-OCH_3)

   - Amine-generating group (NO_3)

   - Other (Br)

RESULTS:
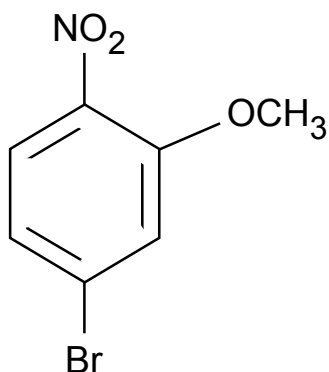
Justification Report is saved in ONCO directory as ASCII file as "Chemical file name.JST"

SUMMARY

Code Number: Amine1

Substance Id: Aromatic Amine#1

The level of *carcinogenicity* concern for this compound is HIGH-MODERATE.

JUSTIFICATION:

In general, the level of *carcinogenicity* concern of an aromatic amine is determined by considering the number or rings, the presence or absence of heteroatoms in the rings; the number and position of amino groups; the nature, number and position of other nitrogen-containing 'amine-generating groups;" and the type, number and position of additional substituents.

Sample Output from OncoLogic Organics
Justification Report (continued)
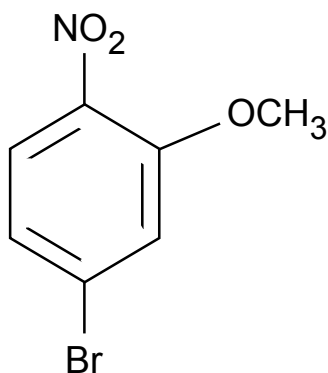
Continued from preceding page

Aromatic amine compounds are expected to be metabolized to N-hydroxylated/N-acetylated derivatives which are subject to further bioactivation, producing electrophilic reactive intermediates that are capable of interaction with cellular nucleophiles (such as DNA) to initiate carcinogenesis.

Nitro groups of aryl compounds can be reduced by nitro reductase to amino groups yielding aromatic amine compounds. The evaluation of this compound proceeds as if the nitro group were a free amine group.

An aromatic compound containing one benzene ring, one amino group, and one methyl or methoxy group ortho- to the amino group, has a *carcinogenicity* concern of HIGH-MODERATE.

The additional chloro and/or bromo group(s) generally raise(s) the level of concern, but they also impose an upper limit of HIGH-MODERATE on the concern level of the compound. Therefore, the level of concern remains HIGH-MODERATE.

The final level of *carcinogenicity* concern for this compound is HIGH-MODERATE.

Notes

ECOSAR to Estimate Aquatic Toxicity

How Does the Model Work?
ECOSAR (Ecological Structure Activity Relationships) estimates the aquatic toxicity of a chemicals used in industry and discharged into water. The program uses Structure Activity Relationships (SARs) to estimate a chemical's acute (short-term) toxicity and, when available, chronic (long-term or delayed) toxicity.

What Does the ECOSAR Model Do?

ECOSAR estimates the aquatic toxicity of a chemical to fish, invertebrates, and algae.

Important Note

ECOSAR (v. 099f) can be downloaded at no cost from EPA, OPPT's New Chemicals Program web site:
http://www.epa.gov/oppt/newchems/21ecosar.htm

ECOSAR User Manual, *ECOSAR: A Computer Program for Estimating the Ecotoxicity of Industrial Chemicals* (EPA-748-R-93-002), and *Estimating Toxicity of Industrial Chemicals to Aquatic Organisms Using Structure Activity Relationships* (EPA-748-R-93-001) can be obtained by calling EPA's National Center for Environmental Publications and Information at 1-800-490-9198.

Why Use the ECOSAR Model?

I need to know the toxicity of the chemical to the plant and animal life in the stream - **Aquatic Toxicity.**

Aquatic Toxicity

Why is Aquatic Toxicity of a Chemical Important?
An understanding of the chemical's aquatic toxicity helps the risk assessor estimate if the release of the chemical will adversely affect biota in the stream or enter the food chain.
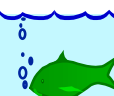
ECOSAR to Estimate Aquatic Toxicity

Important Note

The current version of ECOSAR can not be used to estimate toxicity of certain *chemical classes*, for example: charged dyes, polymers, inorganics, or organometallics.

What You Need to Use ECOSAR

✓ Knowledge of environmental toxicology and organic chemistry
✓ *CAS number* and/or SMILES notation of the chemical
✓ Certain physical/chemical properties of the chemical:
  • Log *KOW* (ClogP*)
  • Melting point

*ClogP vs. log KOW

Most SARs in ECOSAR were developed using *KOW* values predicted using ClogP which is a program developed by BioByte Corp. ClogP values are fairly consistent with EPIWIN's values, however, ClogP values should be entered if available.
BioByte Corp. can be reached at:
Ph: 909-624-5992,
http://www.biobyte.com
All SARs in ECOSAR are being recalculated using EPIWIN's log P values.

Inputs

✓ Chemical structure (SMILES)
✓ Chemical name (optional)
✓ *CAS number* (optional)
✓ Chemical properties (if available)
  • Log *KOW* estimated by ClogP*
  • Melting point
  • Measured water solubility (optional)
  • Measured Log *KOW* (optional)

Outputs

✓ Predicted acute and chronic aquatic toxicity of the chemical (in parts per million)
✓ *Chemical class*

ECOSAR to Estimate Aquatic Toxicity
Data Entry and Results Screens

Ecosar Classes v0.99f

File   Edit   Functions   BatchMode   ShowStructure   Special_Classes   Help

Previous | Get User | Save User | CAS Input | Calculate

Enter SMILES: `c(cccc1)(c1)C`

> Either structure (SMILES) or *CAS number* must be entered to run the program.

Enter NAME: Chemical A

CAS Number:
Chemical ID 1:
Chemical ID 2:
Chemical ID 3:

Measured Water Sol (mg/L): 573.1
Melting Point (deg C): 25.00

Log Kow: 2.540

Measured Log Kow: 2.73

Inputs:
SMILES	c(cccc1)(c1)C
Log Kow	2.540 (ClogP)
Melting Pt	25.0

Ecowin Results

Print   Save Results   Copy   Remove Window

```
SMILES : c(cccc1)(c1)C
CHEM   : Chemical A
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C7 H8
MOL WT : 92.14
Log Kow: 2.54  (User entered)
Melt Pt: 25.00 deg C
Wat Sol: 573.1 mg/L  (measured)

ECOSAR v0.99f Class(es) Found
--------------------------------
Neutral Organics
```

> The results may be Printed, Saved to a file, or Copied to the Windows clipboard and pasted into another Windows Program, such as MS Word.

ECOSAR Class	Organism	Duration	End Pt	Predicted mg/L (ppm)
Neutral Organic SAR (Baseline Toxicity)	: Fish	14-day	LC50	41.891
Neutral Organics	: Fish	96-hr	LC50	21.225
Neutral Organics	: Fish	14-day	LC50	41.891
Neutral Organics	: Daphnid	48-hr	LC50	23.608
Neutral Organics	: Green Algae	96-hr	EC50	15.225
Neutral Organics	: Fish	30-day	ChV	2.983
Neutral Organics	: Daphnid	16-day	EC50	1.533
Neutral Organics	: Green Algae	96-hr	ChV	2.080
Neutral Organics	: Fish (SW)	96-hr	LC50	6.313
Neutral Organics	: Mysid Shrimp	96-hr	LC50	4.163
Neutral Organics	: Earthworm	14-day	LC50	386.488

Results Page from the ECOSAR Model

```
SMILES : c(cccc1)(c1)C
CHEM   : Chemical A
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C7 H8
MOL WT : 92.14
Log Kow: 2.54  (User entered)
Melt Pt: 25.00 deg C
Wat Sol: 573.1 mg/L  (measured)

ECOSAR v0.99f Class(es) Found
-----------------------------
Neutral Organics

                                                      Predicted
ECOSAR Class                 Organism          Duration  End Pt  mg/L (ppm)
==========================   ==================  ========  ======  ==========
Neutral Organic SAR       : Fish                14-day    LC50      41.891
(Baseline Toxicity)

Neutral Organics          : Fish                96-hr     LC50      21.225
Neutral Organics          : Fish                14-day    LC50      41.891
Neutral Organics          : Daphnid             48-hr     LC50      23.608
Neutral Organics          : Green Algae         96-hr     EC50      15.225
Neutral Organics          : Fish                30-day    ChV        2.983
Neutral Organics          : Daphnid             16-day    EC50       1.533
Neutral Organics          : Green Algae         96-hr     ChV        2.080
Neutral Organics          : Fish  (SW)          96-hr     LC50       6.313
Neutral Organics          : Mysid Shrimp        96-hr     LC50       4.163
Neutral Organics          : Earthworm           14-day    LC50     386.488

 Note:   * = asterisk designates: Chemical may not be soluble
         enough to measure this predicted effect.
          Fish and daphnid acute toxicity log Kow cutoff: 5.0
          Green algal EC50 toxicity log Kow cutoff: 6.4
          Chronic toxicity log Kow cutoff: 8.0
          MW cutoff: 1000
```

Inputs:

SMILES	c(cccc1)(c1)C
Log Kow	2.540 (ClogP)
Meas. WS	573.1
Melting Pt	25.0
Meas. Log Kow	2.730

The chronic value (ChV) for fish is 3.0 ppm.

Interpreting the Results from ECOSAR

Standard toxicity profile used by EPA for freshwater species (*mg/L* or ppm):

Acute effects	Duration	Endpoint
fish	96-h	*LC50*
daphnid	48-h	*LC50*
green algae	96-h	*EC50*
Chronic effects	**Duration**	**Endpoint**
fish	30-d	ChV
daphnid	16-d *EC50* or	ChV
green algae		ChV

Establishing ecotoxicity concern levels: Review ACUTE values (lowest value will be most toxic), and use the following criteria:
High = Any of the 3 values are < 1 *mg/L* (Chronic < 0.1 *mg/L*)
Mod. = Lowest of the 3 is > 1 and < 100 *mg/L* (Chronic >0.1 and <10.0 *mg/L*)
Low = All 3 are > 100 (Chronic > 10.0 *mg/L*), or there are No Effects at Saturation (occurs when water solubility of the chemical is higher than an effect concentration).

Determining concern concentration (CC): *CC* is the lowest ChV divided by an uncertainty factor (assessment or safety factor) of 10. In order to be conservative and because the uncertainty (or assessment) factor is one significant digit, the *CC* will be rounded up to be one significant digit e.g., a *CC* of 175 will be rounded up to 200.

Models to Estimate
Exposure and/or Risk

Following are brief fact sheets providing information on the models OPPT uses to estimate the risk to receptors from exposure to chemicals released to the environment. Information provided on each model includes:

- ✓ What exposure/risk property does the model estimate?

- ✓ What is significant about the exposure/risk property to exposure assessment?

- ✓ Why is knowing the exposure/risk property important?

- ✓ Why would I want to use the model?

- ✓ What do I need to run the model?

- ✓ What are the inputs and outputs for the model?

EXPOSURE/RISK MODELS
E-FAST (Now incorporates SEAS, PDM3, Dermal, and SCIES)
ReachScan
Occupational Exposure Spreadsheets
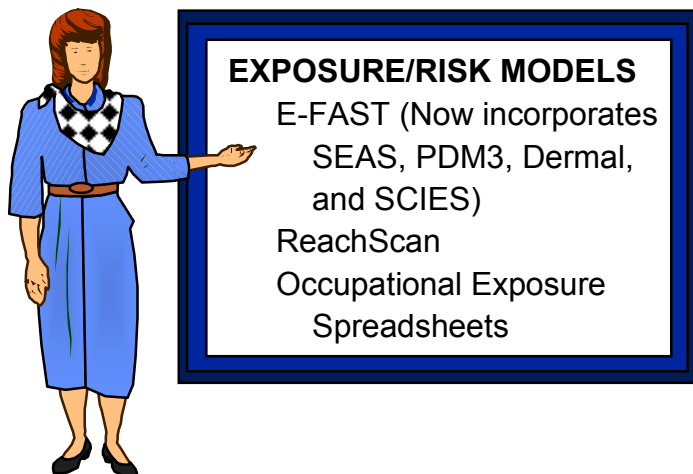
Notes

Exposure, Fate Assessment Screening Tool (E-FAST)

What Is E-FAST?

E-FAST is a Windows based model that incorporates previous DOS based screening level exposure models: SEAS, PDM3, Dermal, and SCIES. E-FAST also incorporates the DOS model FLUSH, which was not previously a part of the P2 Framework.

What Does the E-FAST Model Do?

✓ Provides screening-level estimates of the concentrations of chemicals released to air, surface water, landfills, and from consumer products.
✓ Estimates potential inhalation and ingestion *dose* rates resulting from these releases.
✓ Modeled estimates of concentrations and doses are designed to reasonably overestimate exposures, for use in screening level assessment.

Important Note

The E-FAST Model and documentation manual can be downloaded from the Internet at:
http://www.epa.gov/opptintr/exposure

Check the E-FAST HELP to get information on:
✓ Getting Started
✓ Input Pages for all modules
✓ Results Pages for all modules
✓ References

I need to know if the amount of a chemical released to air, landfills, and surface water may pose a health threat to humans or the aquatic ecosystem.

Why Use the E-FAST Model?

Air, Landfill, SW Conc.

E-FAST: Organized into Four Modules
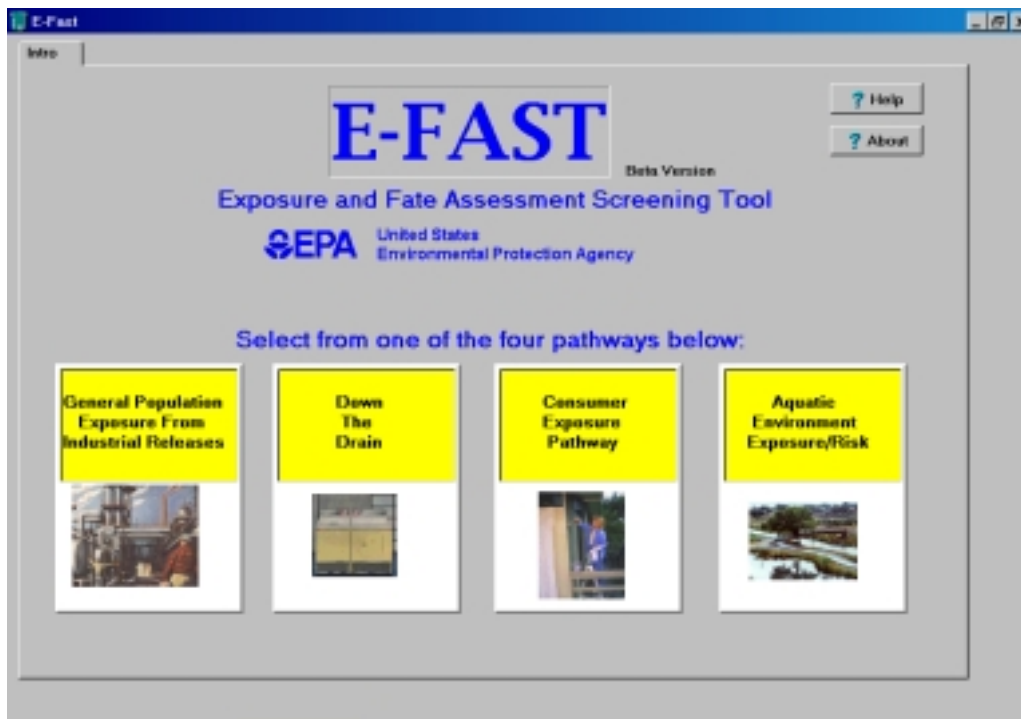
E-FAST is Organized Into 4 Modules:

1. General Population Exposure from Industrial Releases
   (Formerly the model SEAS)

2. Down-the-Drain Residential Releases
   (Formerly the model FLUSH, which was not previously
   a part of the P2 Framework)

3. Consumer Exposure Pathway (CEM)
   (Formerly the models SCIES and Dermal)

4. Aquatic Environment Exposure / Risk
   (Formerly the model PDM3)

E-FAST:
General Population Exposure from Industrial Releases
(Formerly the model SEAS)
Date Entry Screen

Inputs

General Release Information
✓ Release activity (i.e. Industrial Use, Processing);
✓ Number of sites being assessed;
✓ Release media – 4 types are modeled: surface water, landfill, ambient air via incineration, and ambient air via fugitive release;
✓ Release amounts and frequency for each media;
✓ For surface water releases the user will need to determine if the analysis will be site specific or generic (using SIC codes).

Physical Chemical Properties
✓ *Bioconcentration* Factor (*BCF*);
✓ Concentration of Concern (COC);

Exposure Factors
✓ This module has a preset exposure factors for adults, children, and infants (All of the factors can be revised if necessary).

Fate Properties
✓ Wastewater treatment removal;
✓ Drinking water treatment removal;
✓ Percent removal during incineration;
✓ Groundwater migration potential.

E-FAST:
General Population Exposure from Industrial Releases
(Formerly the model SEAS)

Does this Module have any built-in databases?

Yes, these databases are:

✓ Human Exposure Factors;
✓ Site specific surface water discharging facilities (over 55,000 sites accessed by *NPDES* number or company name);
✓ Surface water flow data for 41 industrial SIC codes.

What You Need to Use this E-FAST Module

✓ Chemical-specific data
✓ Release activity data
✓ Site-specific data, such as *NPDES Number*

OR

✓ *SIC* code*

*SIC codes for the 41 industrial activities are provided in later pages of this document.

Outputs

Human Exposure

✓ Drinking water exposure from surface water releases;
✓ Fish ingestion exposure from surface water releases;
✓ Inhalation exposure from fugitive releases;
✓ Inhalation exposure from incineration releases;
✓ Drinking water exposure from landfill releases.

Aquatic Environment

✓ Post-treatment concentration in surface water;
✓ Days per year the *COC* is exceeded;
✓ Percentage of the year the *COC* is exceeded.

Sample Output from E-FAST:
General Population Exposure from Industrial Releases

Click on River Tab and Drinking Water Info to get Human DW Exposure Estimates

Click on River Tab and Fish Ingestion Info to get Human Fish Ingestion Exposure Estimates

Sample Output from E-FAST:
General Population Exposure from Industrial Releases

Click on Incineration Tab to get Incineration Exposure Estimates

Click on Env. Rel.Tab to get Environmental Release Estimates

E-FAST: Down-the-Drain Residential Releases
(Formerly the Flush Model and not previously part of the P2 Framework)

What Does this Module Do?

This module estimates human and aquatic environmental exposure to chemicals released via the use and disposal of certain types of consumer products in a residential setting. This module is designed to assess releases of products that are intended to go down the drain at a home, such as liquid laundry detergent, or bathroom cleaners. Human exposures are estimated for adults, children and infants for releases to surface water. The module also estimates aquatic environmental exposure and risk from surface water releases.

Why Use This Module?

Use this module to assess human drinking water, or fish ingestion exposure to chemicals released during residential down the drain type uses, and to assess the aquatic environment exposure and risk from chemicals released to surface water from residential settings.

Down the Drain

What You Need to Use this E-FAST Module

✓ Chemical-specific data;
✓ Production volume;
✓ Understanding of the consumer product use cycle.

E-FAST: Down-the-Drain Residential Releases

Inputs

✓ Production Volume;
✓ Concentration of Concern;
✓ *Bioconcentration* Factor;
✓ Years in use;
✓ Percent Removal in Wastewater treatment.

Does this Module have any built-in databases?

Yes, these 2 databases are:
✓ Human Exposure Factors;
✓ A generic, United States wide, consumer product use exposure scenario.

Important Note

The HELP screen contains information on running the model QA/QC, Calculations, and References

Down-the-Drain Module
Data Entry Screen

Sample Output from E-FAST:
Down-the-Drain Residential Releases

Outputs

Human Exposure

✓ Drinking water exposure from surface water releases;

✓ Fish ingestion exposure from surface water releases;

Aquatic Environment

✓ Post-treatment concentration in surface water;

✓ Days per year the *COC* is exceeded;

✓ Percentage of the year the *COC* is exceeded.

E-Fast

Intro | Disposal Inputs | *Disposal Res.

Disposal Results   ? Help

Release Activity:	Manufacture	
Production Volume:	1.12E+06	kg/year
WWT Removal:	50.00	%
Release days:	365.00	days
Bio Concentration Factor:	300.00	L/kg

Exposed Population:	Adult	
Median surface water conc:	1.58E-02	ug/L
High end surface water conc:	0.21	ug/L
Pre-treatment release:	1.13E-02	g/person/day
Post-treatment release:	5.64E-03	g/person/day

PDM Information | Drinking Water Information | Fish Ingestion Information

Fish Ingestion Exposure Estimates

Exposure Type	50%ile Res.	10%ile Res.	ED (yrs)	AT (yrs)	BW (kg)	IR (g/day)
Cancer						
LADDpot (mg/kg/day)	1.59E-07	2.06E-06	30.00	75.00	71.80	6.00
LADCpot (mg/kg)	1.90E-03	2.47E-02	30.00	75.00		
Chronic Non-Cancer						
ADDpot (mg/kg/day)	3.96E-07	5.15E-06	30.00	30.00	71.80	6.00
ADCpot (mg/kg)	4.74E-03	6.17E-02	30.00	30.00		
Acute						
ADRpot (mg/kg/day)	8.52E-06	1.11E-04	1 day	1 day	71.80	129.00

Sample Output from E-FAST:
Down-the-Drain Residential Releases

E-FAST: Consumer Exposure Pathway (CEM)
(Formerly SCIES and Dermal)

What Does this Module Do?

This module of E-FAST estimates human inhalation and dermal exposure to chemicals in certain types of consumer products. Human exposures are estimated for adults, and where appropriate children and infants.

Consumer Exposure Pathway (CEM)
Select-a-Scenario Screen
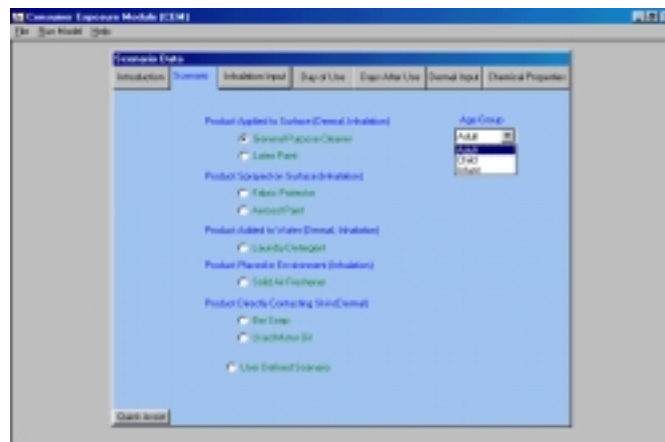
Inhalation (formerly SCIES Model) exposure to:

✓ General purpose cleaners
✓ Latex paint
✓ Fabric protector
✓ Aerosol paint
✓ Laundry detergent
✓ Solid air freshener
✓ User defined "create your own" scenario
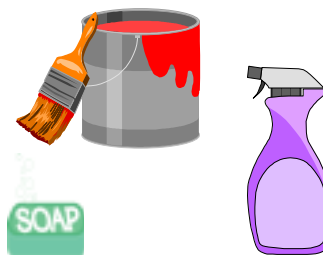
Dermal (formerly Dermal Model) exposure to:

✓ General purpose cleaners
✓ Latex paint
✓ Laundry detergent
✓ Bar soap
✓ Used motor oil
✓ User defined "create your own" scenario

E-FAST: Consumer Exposure Pathway (CEM)
(Formerly SCIES and Dermal)

Inputs

✓ Weight fraction of chemical in consumer product

✓ Molecular weight

✓ Vapor pressure

Does this Module have any built-in databases?

Yes, these databases are:
✓ Human exposure factors;
✓ Default use amounts for 9 preset scenarios;
✓ Activity patterns for residents in the home;
✓ A database of common chemical components of consumer products with associated "typical" weight fractions.

Important Note

The HELP screen contains information on running the model QA/QC, Calculations, and References

What You Need to Use This Module

✓ Chemical-specific data; and,
✓ Understanding of the preset scenario defaults for each scenario.

Why Is Knowing the Potential for Dermal Contact Important?

Knowing the likely dermal *dose* that may occur from using a consumer product helps the risk assessor evaluate the safety of a product prior to its manufacture and use.

Outputs

✓ Concentration of chemical in the indoor environment

✓ Inhalation exposure estimates:
Lifetime Average Daily Dose (*LADD*)
Average Daily Dose (*ADD*)
and Acute Potential Dose Rate (*APDR*)

✓ Dermal exposure estimates:
Lifetime Average Daily Dose (*LADD*)
Average Daily Dose (*ADD*)
and Acute Potential Dose Rate (*APDR*)

E-FAST: Consumer Exposure Pathway
(Formerly SCIES and Dermal)
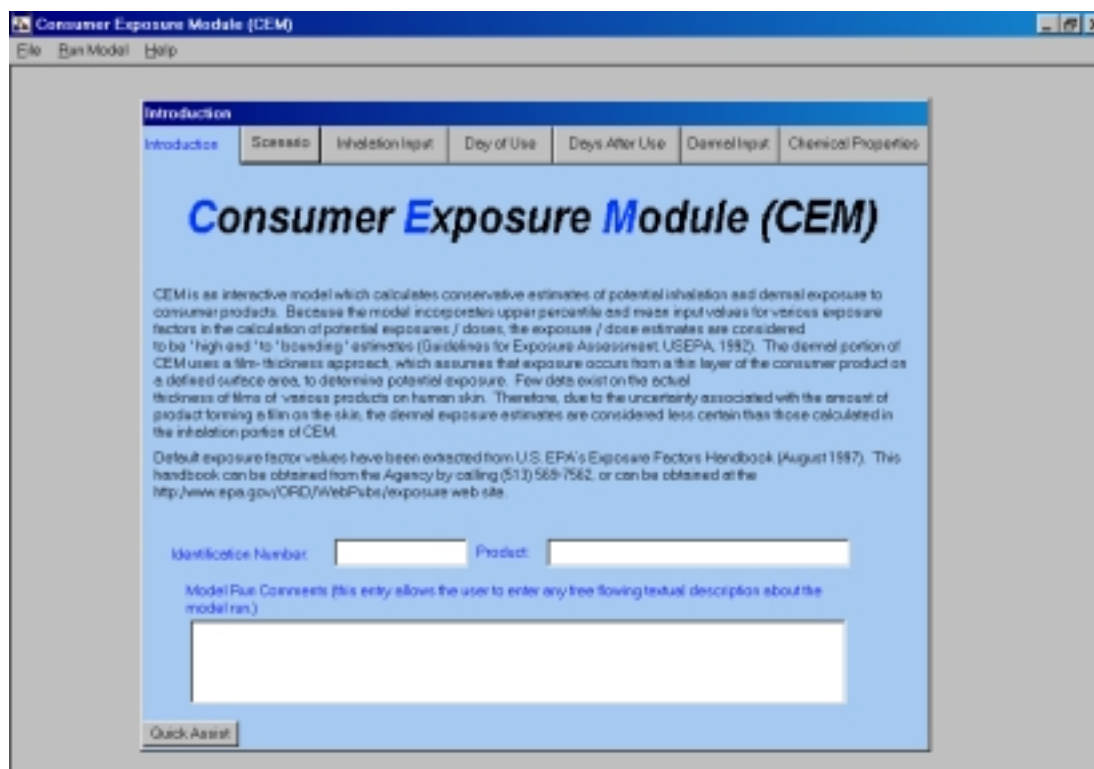
E-FAST: Consumer Exposure Pathway (CEM) Input Screens

Inhalation Scenario Input Screen

Dermal Input Screen

Sample Output from E-FAST:
Consumer Exposure Pathway
(Formerly SCIES and Dermal)

Sample Output from E-FAST:
Consumer Exposure Pathway
(Formerly SCIES and Dermal)

E-FAST: Aquatic Environment Exposure / Risk (Formerly PDM3)

What Is the Aquatic Environment Exposure / Risk Module?

It's a screening-level model that estimates chemical concentration in a stream and can be used with either detailed site-specific data, or more general *Standard Industrial Classification (SIC)* code-based information.

What Does the Aquatic Environment Exposure / Risk Module Do?

This module of E-FAST estimates how many days per year a chemical discharged in a plant's *effluent* will exceed a concentration of concern in the receiving water.

What Is a Concern Concentration (*CC*)?

A *CC* is a concentration level, usually reported in parts per billion (ppb) or parts per million (ppm), which is based on aquatic toxicity data. Harm to the aquatic environment is more likely to occur if the *CC* is exceeded.
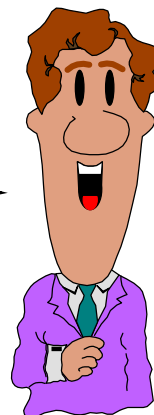
E-FAST: Aquatic Environment Exposure / Risk
(Formerly PDM3)

Why Use This Module?

I need to know if the amount of chemical discharged to a stream will result in stream concentrations that may adversely affect aquatic organisms.

What You Need to Use This Module

- ✓ Inputs required for type of analysis to be conducted (see below), or

- ✓ ECOSAR program - optional (can be used to derive concern concentration *CC*)

Inputs

Site-specific

- ✓ *NPDES* number
- ✓ Release days per year
- ✓ *Loading* - amount released after treatment (kg/day)
- ✓ *CC*

OR

SIC Code-based

- ✓ Analysis choice (usually *high-end* analysis)
- ✓ Standard Industrial Classification (*SIC)* code
- ✓ Release days per year
- ✓ *Loading* - amount released after treatment (kg/day)
- ✓ *CC*

Outputs

✓ Number of days per year the concentration in the stream will exceed the concern concentration (*CC*)

Entry Screen and Sample Output from E-FAST:
Aquatic Environment Exposure / Risk
(Formerly PDM3)

E-Fast					_ □ ×

Intro | *PDM Site | *PDM SIC

Chemical ID:
tmpchem ▼

PDM Site Specific Page | ? Help

NPDES #: MT0000477	<--Find Entered NPDES	Select a NPDES MT0000477 ▼

Release Activity: Unknown   Discharge Type:

Facility name: Company ABC   WWT Removal: 70.00 %

Facility location: BILLINGSMT591031163   Release days: 250.00 days/yr

Reach Number: 10070007039   Concentration of concern: 10.00 ug/L

Reach Name: YELLOWSTONE R   Pre-treatment release: 4.00 kg/day

Facility on reach? ● Yes ○ No ○ Unk.   Post-treatment release: 1.20 kg/day

Mean streamflow: 1.75E+04 MLD

Low streamflow: 1672.50 MLD

Effluent flow: 1.00E-02 MLD

Submit | **Save** | **PDM Site Specific Estimates**

COC (ug/L)	% year exceeded	Days/year exceeded	Rel Days	Pre-treat Load	WWT
10.00	0.01	0.04	250.00	4.00	70.00

Notes

ReachScan to Evaluate Impact of Surface Water Discharges to Drinking Water

What Is ReachScan?

It's a model that estimates a chemical's concentration downstream from the point of discharge, and reports drinking water utilities that have intakes downstream from the discharge point.

What Does the ReachScan Model Do?

ReachScan reports the names of downstream water utilities, their distance from the discharging facility, the number of people those water utilities serve, as well as stream concentrations of the chemical discharged at given distances downstream.

Important Note

ReachScan is an MSDOS model. It will be migrated to Windows as soon as possible, however, it must be installed on a computer operating Windows 3.1 and MSDOS 4.0. It will *not install* on computers operating Windows 95 or 98.

Why Use ReachScan?

ReachScan estimates stream concentration of a facility's discharged chemical at a downstream drinking water utility's intake by one of two methods:
(1) simple dilution, or
(2) accounting for fate processes (degradation).
It can also search for facilities that are up or downstream from a specified facility, water utility, or *reach* (specific river/stream segment).
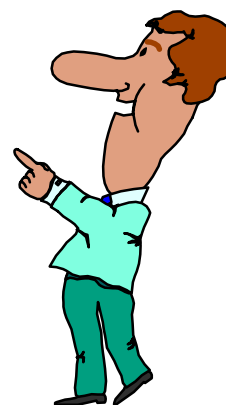
ReachScan to Evaluate Impact of Surface Water Discharges to Drinking Water

Why Do I Need ReachScan?

I need to know what the stream concentration will be of a chemical discharged from my facility at the point where a downstream drinking water utility will use the water.

Inputs

✓ Facility information for the point at which the discharge enters the surface water, including: National Pollutant Discharge Elimination System (*NPDES*) number, name, *SIC* code, or *reach* number

✓ Distance up or downstream to be considered

✓ Amount of chemical released to stream *after treatment* (mg/kg/day)

✓ Chemical properties (molecular weight, solubility, vapor pressure, sorption coefficient (*KOC*), and *half-life*)

✓ If using PDM3: plant *effluent* flow, release days, and concentration of concern

Outputs

✓ Endangered species in the county

✓ PDM3 results (if assessed)

✓ Downstream drinking water utility or facility:

- Chemical concentration at that point
- Population served by water utility
- Distance downstream (km)
- Stream flow at that point

Sample Output from the ReachScan Model

INPUTS:

Hydrologic Region = 02
Search by *NPDES* Number
NPDES Number = PA0027031
Search Query
  Distance of search (KM) = 100
  Downstream
  Utility (drinking water utility)
Endangered Species = Yes
Concentration Parameters
  Loading - amount released after
  treatment (kg/day) = 300
  Consider Environmental Effects
  Flow type* = Mean
Environmental Effects Data
  Chemical name (optional)
    Test chemical
  Molecular weight (g/mol)
    150 <default>**
  Water solubility (ppm)
    100 <default>**
  Vapor pressure (mm-Hg)
    1.0^{-7} <default>**
  Sorption coefficient
    1000 <default>**
  Half-life due to degradation (hrs)
    336
  Suspended solids conc. ppm)
    15.0 <default>**
Environmental Effects / PDM
Analysis :
  Downstream conc. at every
    10 KM
  Dischargers *effluent* flow =
    5.0 MLD
  Number of release days =
    365 days/yr
  Conc. of concern =
    10.0 ppb (or µg/L)

* Mean flow is selected for drinking water concerns; Low flow for aquatic life concerns.

**Program defaults were used to run the model, however data may be entered in place of defaults.

RESULTS:

ReachScan Report   Page 1 of 1

REGION	Region 02			
CALC PARAMETERS	3.000E+02 kg	| Env. Effects : Y	| Mean	
SEARCH PARAMETERS	Downstream	| Utility	| 100.00 km	km Up

SIC	Facility Name		*NPDES*	Reach #	Reach
4952	WEST CHESTER BOROUGH-GOOSE CRE		PA0027031	02040205007	3.86

UTILITY NAME	REACH NUMBER	H C	MEAN FLOW (MLD)	VEL (M/S)	KM DN STREAM	POP SERVED	V C	CONC (µg/L)
WILMINGTON WATER	CO02040205006	Y	1252.37	0.47	30.6	140000	V	2.31E+02
	02040205005		2127.21	0.47	37.6	0		1.35E+02
	02040204060		2139.9	0.47	39.0	0		1.34E+02
	02040204050		47681.18	1.12	59.4	0		6.10E+00
	02040204052		N/A	N/A	LEV 0	0		N/A
	02040204051		N/A	N/A	LEV 0	0		N/A
	02040204046		48284.90	1.12	66.2	0		6.00E+00
	02040204048		N/A	N/A	LEV 0	0		N/A
	02040204047		N/A	N/A	LEV 0	0		N/A
	02040204042		48338.91	1.127	2.8	0		5.97+00
	02040204044		N/A	N/A	LEV 0	0		N/A
	02040204043		N/A	N/A	LEV 0	0		N/A
	02040204039		48510.39	1.13	74.1	0		5.95E+00
	02040204040		N/A	N/A	LEV 0	0		N/A
	02040204036		48590.89	1.13	83.9	0		5.91E+00
	02040204037		N/A	N/A	LEV 0	0		N/A
	02040204033		48852.24	1.13	87.9	0		5.87E+00
	02040204034		N/A	N/A	LEV 0	0		N/A
	02040204029		48912.95	1.13	95.3	0		5.84E+00
	02040204031		N/A	N/A	LEV 0	0		N/A
	02040204030		N/A	N/A	LEV 0	0		N/A

TOT SEARCH DIST.	FINAL REACH	TOT TIME OF TRAVEL	FINAL CONCENTRATION
100.00 KM	02040204025	38.88 HOURS	5.75E+00 µG/L

5/15/97 ReachScan: Environmental Parameters used in search:

Chemical Name:	Test Chemical
Molecular Weight (g / mol)	1.50E+02
Water Solubility (ppm)	1.00E+02
Vapor Pressure (mm / hg)	1.00E-07
Sorption Coefficient	1.00E+03
Chemical *Half-Life* due to Degradation (hours)	3.36E+02
Suspended Solids Concentration (ppm)	1.50E+01

Print Outs from the ReachScan Model

```
ReachScan (PDM) Report                                    Page 1 of 1

REGION              Region 02
CALC PARAMETERS          1.000E+03 kg  | Env. Effects : Y|      Mean
SEARCH PARAMETERS    Downstream         | Utility        |      100.00 km
PDM PARAMETERS           1.00 µg        | 365.00 days    |      5.000E+00 MLD
                                                                          km Up
SIC      Facility Name                             NPDES     Reach        Reach
4952     WEST CHESTER BOROUGH-GOOSE CRE            PA0027031  02040205007  3.86

              MN FLO    LW FLO    LOADING                         KM DN
REACH #       (MLD)     (MLD)     kg          % YEAR   DAYS/YR    STREAM
-----------------------------------------------------------------------------------
02040205006   897.68    366.90    3.80850E-01  11.00    40.15     10.00
02040205006   897.68    366.90    3.80850E-01  11.00    40.15     20.00
02040205006   897.68    366.90    3.80850E-01  11.00    40.15     30.00
02040204050   47681.10  6999.61   1.32574E-02  0.00     0.00      40.00
02040204050   47681.10  6999.61   1.32574E-02  0.00     0.00      50.00
02040204046   48284.72  7033.32   3.68709E-03  0.00     0.00      60.00
02040204042   48338.83  7036.17   1.05845E-03  *.**     *.**      70.00
02040204036   48590.81  7048.94   1.30875E-04  *.**     *.**      80.00
02040204029   48912.87  7067.56   1.53253E-05  *.**     *.**      90.00
02040204025   49541.05  7104.90   2.82970E-06  *.**     *.**      100.00
```

```
Endangered Species Report
-----------------------------------------------------------------------------------
County              :    Chester              State      :    PA
                                              State FIPS :    42
                                              County FIPS :   029
Inventory Name   :  SQUIRREL, DELMARVA PENINSULA FOX
Scientific Name  :  Sciurus niger cinereus
Common Name      :  Delmarva Peninsula Fox Squirrel
Group Name       :  Mammal
Family           :  Sciuridae            Order    :  Rodentia
Status           :  EXN                  Action   :  1
Proposed Date    :
Critical Habit   :                       ESPP     :  N
-----------------------------------------------------------------------------------
County              :    Chester              State      :    PA
                                              State FIPS :    42
                                              County FIPS :   029
Inventory Name   :  BAT, INDIANA
Scientific Name  :  Myotis sodalis
Common Name      :  Indiana bat
Group Name       :  Mammal
Family           :  Vespertilionidae     Order    :  Chiroptera
Status           :  ECN                  Action   :  C
Proposed Date    :  75-12-16
Critical Habit   :  17.95(a)             ESPP     :  N
```

ReachScan Model Flow Diagram

---
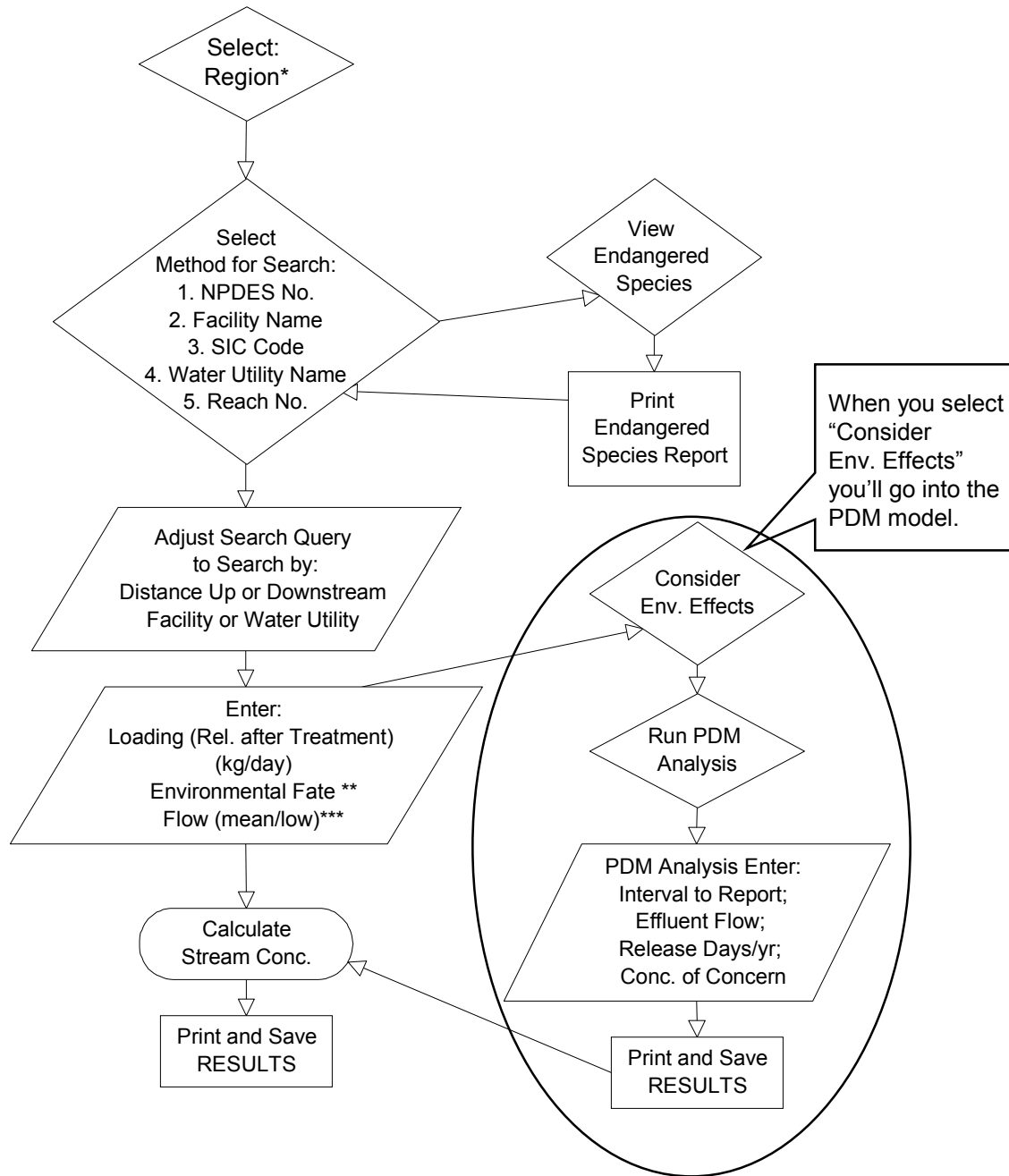
*U.S.G.S. Hydrologic Region of the U.S. A map of the Regions is included in Case Study B, Appendix A.

** If "No" is chosen, the model will calculate concentrations using default values, and predicted concentrations
     may be higher than the actual value.

***For drinking water concerns, select mean flow; for aquatic life concerns, select low flow.

Notes

Occupational Exposure Spreadsheets to Estimate Worker Exposure from Transfer and Open Surface Operations, Textile Dyeing, and Degreasing Operations

What Do These Models Do?

These spreadsheets estimate potential worker *exposure* to:
✓ vapors inhaled during the filling of containers such as drums with liquids or during activities near open pools of liquids;
✓ dust inhaled and/or hand contact with components of dye mixtures used in textile dyeing operations; and
✓ solvent vapors inhaled during degreasing operations.

When Can the Models Be Used?

The transfer/open surface model can be used to estimate *exposure* for a variety of worker activities in variety of industrial settings, including:
✓ Filling tanks or drums with liquids;
✓ Working near an open pool of liquid; and
✓ Sampling liquids.

The other models can be used in specific industrial settings, including:
✓ Textile dyeing; and
✓ Degreasing operations.

How Do the Models Work?

The spreadsheets, developed to run in Lotus123 software, work by combining:
✓ Chemical engineering principles describing the behavior of chemicals;
✓ Default values (can be changed for specific scenarios) for typical industrial processes;
✓ Default values for inhalation rates and dermal contact;
✓ Chemical specific data; and
✓ Scenario specific values for facility operation hours per day, and worker hours per day.

Why Use the Worker Exposure Models?

I need to estimate potential inhalation or Dermal *exposure* of workers during operations using a specific chemical - **Worker Exposure.**

Spreadsheet to Estimate Worker Inhalation Exposure to Vapors from Sampling, Transfer (Filling) Operations and Open Surfaces (Pools) of Liquids

> **What You Need to Use These Worker Exposure Spreadsheets**
> ✓ Chemical specific information
> ✓ Information on operation in which chemical will be used
> ✓ Experience using Lotus spreadsheets (Windows versions)

Required Inputs	Cell No.
✓ Molecular weight	C6
✓ Pure vapor pressure (torr) or partial pressure	C7
✓ Operations hours/day	C8
✓ Worker *exposure* hours/day	C9

Optional Inputs (default values available)	Cell No.
✓ Container volumes	C11-C14
✓ Fill rates	C18-C21
✓ Mixing factors	C25-C26
✓ Inhalation rate	C32
✓ Wind speed	C15
✓ Saturation factors	C22-C24
✓ Ventilation rates	C27-C31
✓ Temperature	C36

Outputs

✓ Inhalation potential dose rate (*PDR*) (mg/day, "typical" and "worst case")

✓ Vapor generation rates (g/sec and kg/day , "typical" and "worst case")

Sample Output from
Spreadsheet to Estimate Worker Inhalation Exposure to Vapors from Sampling, Transfer (Filling) Operations and Open Surfaces (Pools) of Liquids

INPUTS		Cell No.
Molecular weight	250	C6
Vapor pressure	0.1 torr	C7
Hrs/day operations	6	C8
Hrs/day worker *exposure*	6	C9

Exposure and generation rates from transfer operations can be found at cells E44-E54, and from sampling and open surface at cells D60-D77.

RESULTS:

WORKER EXPOSURES AND VAPOR GENERATION RATES FROM TRANSFER OPERATIONS

	Inhalation *Exposure*			Vapor Generation	
	I[mg/day]	Cm[mg/m^3]	Cv[ppm]	G[g/sec]	G[kg/day]
Drumming (55 gal)					
Worst Case	7.32E+02	9.76E+01	9.54E+00	2.35E-03	5.09E-02
Typical Case	8.13E+00	1.08E+00	1.06E-01	7.85E-04	1.70E-02
Cans/Bottles (5 gal)					
Worst Case	6.62E+01	8.83E+00	8.63E-01	2.13E-04	4.60E-03
Typical Case	7.36E-01	9.81E-02	9.59E-03	7.10E-05	1.53E-03
Tank Truck (5,000 gal)					
Worst Case	1.67E+01	2.23E+00	2.18E-01	1.42E-02	3.07E-01
Typical Case	1.86E+00	2.48E-01	2.42E-02	1.42E-02	3.07E-01
Tank Car (20,000 gal)					
Worst Case	3.34E+01	4.46E+00	4.36E-01	2.84E-02	6.13E-01
Typical Case	3.72E+00	4.95E-01	4.84E-02	2.84E-02	6.13E-01

WORKER EXPOSURES AND VAPOR GENERATION RATES DUE TO SAMPLING AND OPEN SURFACE

	Inhalation Exposure			AREA	DIAMETER			Vapor Generation	
Sampling	I[mg/day]	Cm[mg/m^3]	Cv[ppm]	A[cm^2]	z[cm]	Q[ft3/min]	k	G(g/sec)	G(kg/day)
Worst Case	4.47E+01	5.96E+00	5.83E-01	7.85E+01	1.00E+01	5.00E+02	1.00E-01	1.44E-04	3.11E-03
Typical Case	7.48E-01	9.97E-02	9.75E-03	3.85E+01	7.00E+00	3.50E+03	5.00E-01	8.42E-05	1.82E-03
Open surface									
Worst Case	1.24E+03	1.65E+02	1.61E+01	6.58E+03	9.15E+01	5.00E+02	1.00E-01	3.98E-03	8.59E-02
	6.73E+02	8.98E+01	8.78E+00	2.92E+03	6.10E+01	5.00E+02	1.00E-01	2.17E-03	4.68E-02
	2.38E+02	3.17E+01	3.10E+00	7.31E+02	3.05E+01	5.00E+02	1.00E-01	7.66E-04	1.65E-02
	8.41E+01	1.12E+01	1.10E+00	1.83E+02	1.53E+01	5.00E+02	1.00E-01	2.71E-04	5.85E-03
	2.96E+01	3.95E+00	3.86E-01	4.54E+01	7.60E+00	5.00E+02	1.00E-01	9.52E-05	2.06E-03
	1.62E+01	2.16E+00	2.11E-01	2.03E+01	5.08E+00	5.00E+02	1.00E-01	5.21E-05	1.12E-03
	5.72E+00	7.63E-01	7.46E-02	5.07E+00	2.54E+00	5.00E+02	1.00E-01	1.84E-05	3.97E-04
Typical Case	4.12E+01	5.50E+00	5.38E-01	6.58E+03	9.15E+01	3.00E+03	5.00E-01	3.98E-03	8.59E-02
	2.24E+01	2.99E+00	2.93E-01	2.92E+03	6.10E+01	3.00E+03	5.00E-01	2.17E-03	4.68E-02
	7.93E+00	1.06E+00	1.03E-01	7.31E+02	3.05E+01	3.00E+03	5.00E-01	7.66E-04	1.65E-02
	2.80E+00	3.74E-01	3.66E-02	1.83E+02	1.53E+01	3.00E+03	5.00E-01	2.71E-04	5.85E-03
	9.87E-01	1.32E-01	1.29E-02	4.54E+01	7.60E+00	3.00E+03	5.00E-01	9.52E-05	2.06E-03
	5.39E-01	7.19E-02	7.03E-03	2.03E+01	5.08E+00	3.00E+03	5.00E-01	5.21E-05	1.12E-03
	1.91E-01	2.54E-02	2.49E-03	5.07E+00	2.54E+00	3.00E+03	5.00E-01	1.84E-05	3.97E-04

Spreadsheet to Estimate Worker Exposures from Textile Dyeing

When Can the Model Be Used?

This model can be used to estimate *exposure* from batch or continuous operations where less than 54 kg of powered or liquid textile dye is weighed per day. If the dye is in liquid form and vapor pressure exceeds 0.001 torr, the Transfer/Open Surface Model should be used.

Batch and Continuous Operations

INPUTS

✓ Pounds fiber/lot

✓ Percent formulated dye weight/fabric weight

✓ Percent dye strength

✓ Number of machines/site

✓ Number of shifts of operation/day

✓ Number of kilograms purchased/site

✓ Annual production/import vol. of chemical in dye

✓ Percent degree of dye exhaustion

✓ Number of dye weighings/lot (worst case)

✓ Number of dye weighings/lot (typical case)

✓ Liquor ratio (Batch Operations only)

✓ Percent wet pick-up (Continuous Operations only)

✓ Number of machines/machine operator

✓ Number of dye weighers/shift

Important Note

Default values (found in cells R4 through R33) are available for all input variables except annual production or import volumes. Each default value should be reviewed. If actual scenario-specific values are available for any of these variables, they should be entered instead of using the default values.

Default values are presented on the following page.

Outputs

✓ Inhalation potential dose rates (*PDRs*) (mg/day, "typical" and "worst case")

✓ Number of facilities and workers exposed, and number of days of worker *exposure*

✓ Dermal potential dose rates (*PDRs*) (mg/day)

Spreadsheet to Estimate Worker Exposures from Textile Dyeing

Input Variables and the Default Values

INPUT VARIABLES

Cell No.	DEFAULTS	BATCH OPERATIONS
R4	1000	pounds fiber per lot (1000 lbs)
R5	2.5	% formulated dye on weight of fabric (owf) (0.1-5)
R6	58	% dye strength (liq. 10-40; pdwr = 20-60)
R7	4	number of machines per site (1-20 mach. with 4 typical)
R8	3	number of shifts of operation/day (2 or 3)
R9	1000	number of kilograms purchased per site (1000 kilos)
R10	0	PV or IV (in kgs)
R11	0	% degree of exhaustion (60-99)
R12	3	number of dye weighings per lot (worst case) (3)
R13	1.5	number of dye weighings per lot (average case) (1.5)
R14	20	liquor ratio (12-25; typically 20)
R15	2	number of machines per machine operator (2)
R16	1	number of dye weighers/shift (1)

CONTINUOUS OPERATIONS

Cell No.	DEFAULTS	CONTINUOUS OPERATIONS
R21	3600	pounds fiber per lot (3600 lbs)
R22	2.5	% formulated dye owf (0.1-5)
R23	50	% dye strength (liq. 10-40; pdwr = 20-60)
R24	1	number of machines per site (1-5 mach. with 1 typical)
R25	3	number of shifts of operation/day (2 or 3)
R26	1000	number of kilograms purchased per site (1000 kilos)
R27	0	PV or IV (in kgs)
R28	0	% degree of fixation (75-99)
R29	4	number of dye weighings per lot (worst case) (4)
R30	2	number of dye weighings per lot (average case) (2)
R31	80	% wet pick-up (80-200; typically 80)
R32	2	number of machine operators per machine (2)
R33	1	number of dye weighers/shift (1)

Sample Output from Spreadsheet to Estimate Worker Exposures from Textile Dyeing

The results presented here are based on default values (see previous page). There were no scenario-specific inputs for this model run.

OUTPUT

SUMMARY OF RESULTS

Cell No.	DEFAULTS	**BATCH OPERATIONS**
I8	75	total number of dye weighers
I9	9	number of days *exposure*
I10	25	number of sites
I11	2.9175	mg/day average case inhalation *exposure*
I12	9.8473	mg/day worst case inhalation *exposure*
I13	377 - 1131	mg/day Dermal *exposure*
I14	150	total number of machine operators
I15	30 - 89	mg/day Dermal *exposure*
I16	21.09	kilograms per site-day released
I17	9	number of days of release
I18	25	number of sites
I19	4745.45455	kilograms total releases to water

Cell No.	DEFAULTS	**CONTINUOUS OPERATIONS**
I22	6	total number of dye weighers
I23	12	number of days *exposure*
I24	2	number of sites
I25	1.9514	mg/day average case inhalation *exposure*
I26	6.5864	mg/day worst case inhalation *exposure*
I27	325 - 975	mg/day Dermal *exposure*
I28	12	total number of machine operators
I29	46 - 209	mg/day Dermal *exposure*
I30	15.13	kilograms per site-day released
I31	12	number of days of release
I32	2	number of sites
I33	363	kilograms total releases to water

Spreadsheet to Estimate Worker Exposures from Degreasing Operations

When Can the Model Be Used?

This model can be used to estimate inhalation *exposure* from volatile liquid solvents used in two types of vapor degreasing unit operations

1. Open top vapor degreasing (OTVD)
2. Conveyorized or in-line degreasing

Required Inputs	Cell No.
✓ Production/import volume (kg/yr)	C3
✓ Molecular weight	C4

Important Note

The primary default values used by the model should be reviewed and if actual scenario- specific values are available, these should be entered instead of using the default values. The primary default values which should be checked include:

Small and medium batch cleaners: idling 6 hr/day, working 2 hr/day, down 16 hr/day for 260 days/yr; down 24 hr/day for 105 days/yr.

Large and very large batch cleaners: idling 2 hr/day, working 6 hr/day, down 16 hr/day for 260 days/yr; down 24 hr/day for 105 days/yr.

Conveyorized In-line cleaners: idling 0 hr/day, working 8 hr/day, down 16 hr/day for 260 days/yr; down 24 hr/day for 105 days/yr.

Outputs

✓ Estimated numbers of sites and workers

✓ Days per year of *exposure*

✓ Annual emissions in kg/yr

✓ Inhalation potential dose rate (mg/d, "routine" and "bounding")

Sample Output from Spreadsheet to Estimate Worker Exposures from Degreasing Operations

"Routine" and "bounding" Potential Dose Rate results can be found at cells G101-G114 and H101-H114, respectively.

INPUTS:	Cell No.
PV=10,000,000 (kg/yr)	C3
MW = 200	C4

RESULTS:

SUMMARY OF AIR EMISSIONS FOR VAPOR DEGREASING SCENARIO

Scenario		Estimated # of Sites	Estimated Release Days/yr	Annual Emissions (kg/year)
Uncontrolled				
Batch OTVD	Small	94	260	7900
	Medium	26	260	14500
	Large	12	260	40200
	Very Large	7	260	78100
Conveyorized		5	260	49800
Controlled				
Batch OTVD	Small	25	260	7100
	Medium	39	260	13600
	Large	39	260	34000
	Very Large	32	260	66200
Conveyorized		126	260	19900
--				
TOTAL		410		9064000

SUMMARY OF INHALATION EXPOSURES FOR VAPOR DEGREASING SCENARIO

Scenario		Estimated # of Wkrs	Potential Dose Rate Routine	Bounding	Duration
Uncontrolled					
			(mg/d)	(mg/d)	(days/yr)
Batch OTVD	Small	280 - 850	1,000	31,000	260
	Medium	77 - 230	2,000	66,000	260
	Large	34 -104	5,000	163,000	260
	Very Large	21 - 64	11,000	316,000	260
Conveyorized		13 - 41	11,000	324,000	260
Controlled					
Batch OTVD	Small	75 - 175	600	18,400	260
	Medium	117 - 275	1,000	39,800	260
	Large	117 - 274	3,000	98,000	260
	Very Large	96 - 225	6,000	190,000	260
Conveyorized		378 - 883	4,320	130,000	260
--					
TOTAL		1200 - 3100			260

Notes

Notes

Computer Requirements
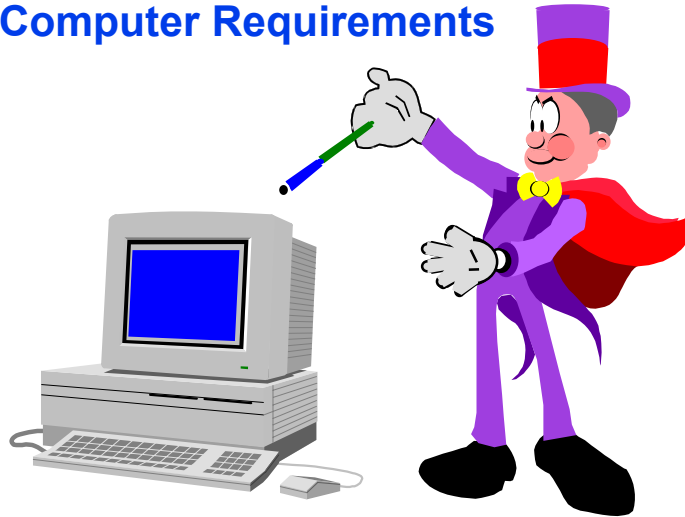
EPI Suite:
- ✓ IBM-compatible PC with Microsoft Windows 3.1, 95, 98, 2000 and Windows NT, a mouse (not required, but highly recommended),
- ✓ EPI Suite (all individual estimation programs and their help files) requires approximately 10 MB of hard disk space
- ✓ 10 MB of hard disk space for SMILECAS

OncoLogic
- ✓ 386 PC with MS-DOS 5.0 or later, a mouse, and color monitor
- ✓ 570K of conventional RAM
- ✓ 60 megabytes of hard disk space
- ✓ A disk cache will significantly improve performance

ECOSAR
- ✓ IBM-compatible PC with a 640-KB memory, 512-550 KB of free memory, and 80386 or 80286 processor
- ✓ MS Windows 3.1, 95, 98, or NT
- ✓ Expanded memory and disk cache will improve performance
- ✓ At least 51 file handlers specified in your CONFIG.SIS file

E-FAST
- ✓ PC with Windows 95, 98, or NT, plus printer and mouse
- ✓ 486 Processor, Pentium or faster is recommended
- ✓ 16 megabytes of memory
- ✓ 48 megabytes of hard disk space
- ✓ SVGA Monitor 800 x 600, color setting on High color (16 bit)
- ✓ WordPerfect 6.1 - 8.0 software is needed to create reports

ReachScan
- ✓ PC with MS-DOS 3.0 or higher, color monitor, and printer
- ✓ 640K of memory
- ✓ 18 megabytes of hard disk space
- ✓ Will not install on computers with Windows 95 or higher

Occupational Spreadsheets
- ✓ PC with Windows 3.1 or higher, SVGA color monitor with 800 x 600 resolution, and printer, Lotus123, Vers. 4.0 or higher
- ✓ 4 megabytes of memory
- ✓ 8 megabytes of hard disk space

SIC Codes for 41 Industries

INDUSTRY	Standard Industrial Classification (SIC) Code(s)
1 Adhesives and Sealants Manufacture	2891
2 Auto and Other Laundries	7211, 7213-7219, 7542
3 Can (metal) Manufacture	3411
4 Dyes and Pigments Manufacture	2865
5 Electronic Components Manufacture	3674, 3679
6 Electroplating	3471
7 Foundries	332, 336
8 Ink Formulation	2983
9 Inorganic Chemicals Manufacture	281
10 Large Household Appliances and Parts Manufacture	3631-3633, 3639, 3431, 3469
11 Leather Tanning and Finishing	3111
12 Lubricant Manufacture	2911, 2992
13 Manufacture of Photographic Equipment and Supplies	7221, 7333, 7395, 7819
14 Metal Finishing	3411-62, 3465-71, 3482-3599, 3613-23, 3629, 3634-6, 3643-51, 3661-71, 3673, 3676-8, 3693-4, 3699, 3711-3841, 3851, 3873-999
15 Motor Vehicle Manufacture	3711, 3713
16 Organic Chemicals Manufacture	2865, 2869
17 Ore Mining and Dressing	101-109
18 Paint Formulation	2851
19 Paper and Paperboard Mills	2621, 2631, 2661
20 Paper Mills except Building Paper Mills	2621
21 Paper Board Mills	2631
22 Building Paper and Board Mills	2661
23 Pesticides Manufacture	2819, 2869, 2879
24 Petroleum Refining	2911
25 Photographic Processing	7221, 7333, 7395, 7819
26 Plastic Products Manufacture	3079
27 Plastic Resins and Synthetic Fabrics	2821, 2823, 2824
28 POTWs (Industrial)	4952
29 POTWs (All Facilities)	4952
30 Primary Metal Forming Manufacture	3315-17, 3351-57, 3463, 3497
31 Printing	271-277
32 Pulp Mills	2611
33 Rubber Products Manufacture	3011, 3021, 3031, 3041
34 Soaps, Detergents, etc. Manufacture	2841-44
35 Steam Electric Power Plants	4911
36 Textile Dyeing and Finishing (Carpets)	2271-72, 2279
37 Textile Dyeing and Finishing (Knit Goods)	225, 2292
38 Textile Dyeing and Finishing (Wool Goods)	2231
39 Textile Dyeing and Finishing (Woven Goods)	2261-62, 2269
40 Textile Dyeing and Finishing (Knit, Wool, and Woven Goods)	2231, 2250, 2269, 2292
41 Yarn and Thread Mills	2281-84

Glossary of Useful Terms

7Q10 flow: Lowest 7-consecutive day average stream flow over a 10 year period (used to assess chronic risks to aquatic live).

Acute toxicity: Adverse effects on any living organism that results from a single dose or single exposure of a chemical; any poisonous effect produced within a short period of time, usually less than 96 hours.

ADD (Average daily dose): The estimate of dose averaged over the number of years of use/exposure to the chemical; used in assessments of risk of non-cancer chronic health effects.

APDR (Acute potential dose rate): The estimated dose on a given day; used in assessments of the risk of acute toxic effects.

BCF: Bioconcentration factor (BCF) is the ratio (in L/kg) of a chemical's concentration in the tissue of an aquatic organism to its concentration in the ambient water. BCF indicates the potential for the chemical to concentrate in lipids (fats) of organisms.

Bioaccumulation: Process in which lipid soluble chemicals are stored in fatty tissue (lipids) of organisms and can increase in concentration over time.

Bioassay: Testing method that measures the effects of a material on living organisms.

Bioconcentration: Bioaccumulation of lipid soluble chemicals in fatty tissues (lipids) of organisms at concentrations higher than that of the surrounding water.

Biodegradable: Ability of a substance to be broken down physically and/or chemically by microorganisms.

Biomagnification: Process in which lipid soluble substances increase in fatty tissues (lipids) of organisms higher in the food web as contaminated food species are consumed.

Carcinogen(ic): Ability of a substance to cause cancer.

Chemical Abstract Service (CAS): Organization which assigns unique numbers to chemical substances submitted to them. CAS Registry Numbers are the unique identifier for a chemical substance, while chemical names may not be unique.

Chemical class: The general chemical group to which a chemical belongs (e.g., acid, base, hydrocarbon, etc.).

Chronic Toxicity: Adverse effects on any living organism in which symptoms develop slowly over a period of time (often the life time of the organism) or reoccur frequently.

Concern concentration (CC) or Concentration of Concern (COC): Reported in parts per billion (ppb) or parts per million (ppm), provides the concentration of a chemical in a stream and indicates the concentration at which harm is more likely to occur to aquatic organisms. CC is determined by dividing the lowest chronic toxicity value by 10.

Direct discharge: Under NPDES permitting, the discharge of chemicals or compounds directly to a surface water body.

Dose: In terms of monitoring exposure levels, the amount of a toxic substance taken into the body over a given period of time.

Dose Response: The manner in which an organism's response to a toxic substance changes as its overall exposure to the substance changes.

EC50 (Effective Concentration 50): Median effective concentration is the concentration of a pollutant at which 50% of the test organisms die; a common measure of acute toxicity.

Effluent: The stream flowing out of a facility or water body. The concentrations in it's flow are used to estimate potential health effects of the discharge.

Exposure: Pollutants that come in contact with the body and present a potential health threat, via inhalation, ingestion, or dermal routes. The route, magnitude, and duration of exposure contributes to the ultimate risk for the organism.

Half-life: Time required for one-half of a chemical or compound to degrade.

Glossary of Useful Terms (continued)

Harmonic mean: The number of daily flow measurements divided by the sum of the reciprocals of the flows. A value that is more conservative than the arithmetic mean flow value. Used to assess chronic risks to humans.

Hazard: Potential for a substance to cause adverse effects to organisms, for example birth defects.

High end: A plausible estimate of an individual exposure or dose for those persons at the upper end of an exposure or dose distribution, above the 90th percentile, but no higher than the individual in the population who has the highest exposure.

Hydrophilic: Having an affinity for, or capable of dissolving in, water.

Influent: Stream flowing into a facility or water body.

Indirect discharge: Under NPDES permitting, unlike a direct discharger, an indirect discharger from a nonresidential source pumps effluent to another facility that has a permit to discharge to the stream. Indirect dischargers often pretreat their discharges prior to pumping them to the publicly owned treatment works.

KOC: Organic carbon partition coefficient - the ratio of amount of a chemical adsorbed per unit weight of organic carbon to the chemical concentration in solution at equilibrium Is an indication of how the chemical will partition itself between the solid and solution phases of a water-saturated or unsaturated soil.

KOW: Octanol-water partition coefficient - the ratio of a chemical's concentration in the octanol phase to it's concentration in the aqueous phase of a two-phase octanol/water system.

LADD (Lifetime average daily dose): The estimated dose to an individual averaged over a lifetime of 70 years; used in assessments of *carcinogenic* risk.

LC50 (Lethal Concentration 50): Median lethal concentration is the concentration of a pollutant at which 50% of the test organisms die; a common measure of acute toxicity.

LD50 (Lethal Dose 50): The dose of a toxicant that will kill 50% of test organisms within a designated period of time. The lower the LD50, the more toxic the compound.

Lipophilic: Having an affinity for, or capable of dissolving in, fat and fatty materials.

Loading: The amount of chemical that is discharged to a stream after treatment, reported in kg/day.

Milligrams/liter (mg/L): A measure of concentration used in the measurement of fluids that is roughly equivalent to parts per million.

Moiety(ies): Compounds formed when a larger compound is subdivided.

MSDS (Material Safety Data Sheet): Printed material concerning a hazardous chemical including its physical properties, hazards to personnel, fire and explosive potential safe handling and transportation recommendations, health effects, reactivity, and proper disposal. Originally established for employee safety by OSHA.

Mutagenicity: The property of a chemical to cause genetic mutations that are expressed in the next generation but not necessarily in the organism exposed to the mutagen.

No Observed Adverse Effect Level (NOAEL) or No Observed Effect Level (NOEL): Level of exposure which does not cause observable harm.

NPDES (National Pollutant Discharge Elimination System): is the primary permitting program under the Clean Water Act which requires that dischargers of chemicals to surface waters obtain a permit from EPA. A NPDES permit number is a nine-character number with the two letter State abbreviation beginning the number (e.g., NC0001234).

Parts per billion (ppb): One ppb is comparable to one kernel of corn in a filled, 45-fool silo, 16 feet in diameter.

Parts per million(ppm): One ppm is comparable to one drop in the gasoline tank of a full-size car.

Parts per trillion (ppt): One ppt is comparable to one drop in a swimming pool the size of a football field and 43 feet deep.

Glossary of Useful Terms (continued)

Permissible Exposure Limit (PEL): Workplace exposure limits for contaminants established by OSHA.

Point Source: A stationary location or fixed facility such as an industry or municipality that discharges pollutants into air or surface water.

Pollution: Any substances in environmental media that degrade the natural quality of the environment.

Pollution Prevention (P2): The concept stating that it is easier to <u>prevent</u> pollution than to clean up pollution after it has occurred.

Potential Dose Rate(s) PDR(s): Provide an estimate of possible exposure rate to receptor from expected use, usually derived by modeling using default exposure factors.

POTW (Publicly Owned Treatment Works): A municipal or public service district sewage treatment system.

Reach: A reach is a stream or river segment identified by EPA and assigned an 11-digit identification number. The first two numbers indicate the hydrologic region of the United States in which the reach is located.

Reference Dose (RfD): The particular concentration of a chemical that is known to cause health problems.

Release: Any spilling, leaking, pumping, pouring, emitting, emptying, discharging, injecting, escaping, leaching, dumping, or disposing into the environment of a hazardous or toxic chemical.

Risk: A measure of the chance that damage to life, health, property, or the environment will occur.

Risk Assessment: A process to determine the increased risk from exposure to environmental pollutants together with an estimate of the severity of impact. Risk assessments use specific chemical information plus risk factors.

SARs: Structure Activity Relationship (SAR) predict the toxicity of chemicals based on their structural similarity to chemicals for which toxicity data are available. SARs express the correlations between a compound's physicochemical properties and its toxicity. SARs measured for one compound can be used to predict the toxicity of similar compounds belonging to the same chemical class. EPA routinely uses to estimate toxicity of chemicals submitted as Pre-Manufacture Notices mandated by Section 5 of the Toxic Substances Control Act (TSCA).

SIC Code: Standard Industrial Classification Code system is a four digit number that identifies the specific industrial activity. For a complete listing of SIC codes, see   Standard Industrial Classification Manual. 1987. Supt. of Documents, U.S. Government Printing Office, Washington, DC.

Toxicity Testing: Biological testing (usually with an invertebrate, fish, or small mammal) to determine the adverse effects, if any, of a chemical substance.

Notes

APPENDIX A

Case Studies

Case Study A - **Potential Aquatic and Human
Exposures to Surface Water Discharges
from a Manufacturing Facility**
Uses the Models ECOSAR and the E-FAST
General Population Exposure from Industrial
Releases Module

Case Study B - **Potential Exposures to Surface Water
Discharges from a Manufacturing Facility**
Uses the Models PCKOCWIN and ReachScan

Case Study C - **Consumer Dermal Exposure**
Uses the E-FAST Consumer Exposure Pathway
(CEM) Module

Case Study D - **Worker Inhalation Exposure**
Uses the Occupational Exposure Spreadsheets
to Estimate Worker Exposure

Notes

Case Study A

Potential Aquatic and Human Exposures to Surface
Water Discharges from a Manufacturing Facility

Uses the Models ECOSAR and the E-FAST
General Population Exposure from Industrial Releases Module
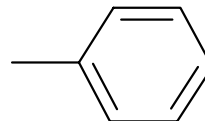
Notes

CASE STUDY A
Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Introduction

The purpose of this case study is to determine the aquatic toxicity of Chemical A and to assess potential aquatic impacts and human exposures that may occur as a result of *effluent* discharges from the manufacturing facility (Company ABCDE) in Smalltown, New York. The following models will be used to accomplish this task: ECOSAR and E-FAST: General Population Exposure from Industrial Releases module.

- ECOSAR will be used first to estimate a *concern concentration* for the chemical.
- E-FAST will then be used to estimate the surface water concentration and the likelihood of potential impacts.

Chemical A (structure at right) is a compound in the neutral organic chemical class. No significant aquatic toxicity testing has been done on Chemical A.

Step 1. Toxicity Determination

Because no aquatic toxicity data are available for Chemical A, ECOSAR will be used to predict its aquatic toxicity based on structural similarities to other neutral organic chemicals. The following physical/chemical properties will be assumed for Chemical A that are inputs to run the ECOSAR and E-FAST models:

- measured water solubility = 573.1 *mg/L*;
- melting point = 25° C;
- log *KOW* = 2.540 (ClogP);
- measured log *KOW* = 2.730; and
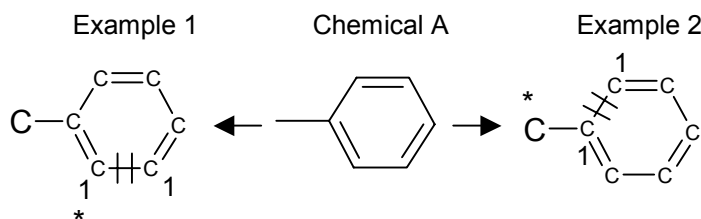- fish *BCF* = 175 (not log BCF).

CASE STUDY A
Potential Aquatic and Human Exposures to Surface
Water Discharges from a Manufacturing Facility (continued)

Running ECOSAR

Since you have no *CAS Number* for Chemical A, you will need to write SMILES notation to run ECOSAR. For help in writing SMILES see Appendix C or the Help screen in ECOSAR. There are many correct ways to write SMILES for a given chemical. Two examples are given below.

Start the SMILES string at the "***".

Example 1 SMILES = c1c(C)cccc1   Example 2 SMILES = Cc1ccccc1

Open ECOSAR and select "All Others" Chemicals group. Enter measured data and SMILES notation (Figure A1), then click on Calculate button. Figure A2 presents the results of running the model.

Figure A1
ECOSAR Data Entry Screen

CASE STUDY A
Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Figure A2
Results of Running ECOSAR

```
SMILES : c1c(C)cccc1
CHEM   : Chemical A (run using SMILES Example 1)
CAS Num:
ChemID1:
ChemID2:
ChemID3:
MOL FOR: C7 H8
MOL WT : 92.14
Log Kow: 2.54  (User entered)
Melt Pt: 25.00 deg C
Wat Sol: 573.1 mg/L  (measured)

ECOSAR v0.99f Class(es) Found
-----------------------------
Neutral Organics


                                                       Predicted
ECOSAR Class               Organism           Duration End Pt  mg/L (ppm)
========================== ================== ======== ======  ==========
Neutral Organic SAR        : Fish             14-day   LC50      41.891
(Baseline Toxicity)

Neutral Organics           : Fish             96-hr    LC50      21.225
Neutral Organics           : Fish             14-day   LC50      41.891
Neutral Organics           : Daphnid          48-hr    LC50      23.608
Neutral Organics           : Green Algae      96-hr    EC50      15.225
Neutral Organics           : Fish             30-day   ChV        2.983
Neutral Organics           : Daphnid          16-day   EC50       1.533
Neutral Organics           : Green Algae      96-hr    ChV        2.080
Neutral Organics           : Fish  (SW)       96-hr    LC50       6.313
Neutral Organics           : Mysid Shrimp     96-hr    LC50       4.163
Neutral Organics           : Earthworm        14-day   LC50     386.488

 Note:  * = asterisk designates: Chemical may not be soluble
        enough to measure this predicted effect.
         Fish and daphnid acute toxicity log Kow cutoff: 5.0
         Green algal EC50 toxicity log Kow cutoff: 6.4
         Chronic toxicity log Kow cutoff: 8.0
         MW cutoff: 1000
```

Inputs:
SMILES	
Chemical Name	
Log *Kow* (ClogP)	2.540
Meas. WS	573.1
Melting Pt	25.0
Meas. Log Kow	2.730

Note: The standard toxicity profile used by EPA for freshwater species is:

Acute Effects:	Fish	96-hr *LC50* (*mg/L*)
	Daphnid	48-hr *LC50*
	Green algal	96-hr *EC50*
Chronic Effects:	Fish	ChV
	Daphnid	ChV or 16d *EC50*
	Green algal	ChV

Chemical A Aquatic Toxicity Profile is: *mg/L*

Acute Effects:	Fish	96-hr *LC50*	22.0
	Daphnid	48-hr *LC50*	24.0
	Green algal	96-hr *EC50*	15.0
Chronic Effects:	Fish	ChV	3.0
	Daphnid	ChV	1.5
	Green algal	ChV	2.0

CASE STUDY A
Potential Aquatic and Human Exposures to Surface
Water Discharges from a Manufacturing Facility (continued)

Determine *Concern Concentration*

The next step is translating the predicted endpoints into a freshwater (FW) *concern concentration* (CC). The following equation is used to calculate the FW CC. The lowest chronic value, the predicted endpoint for Daphnid (1.5 *mg/L* or ppm), was used. An uncertainty factor (assessment or safety factor) is 10 was used to account for the uncertainty of laboratory to field variation, and as a margin of safety.

(Predicted Endpoint x 1,000 conversion from ppm to ppb) / safety factor

(1.5 ppm x 1,000) / 10 = 150 ppb, rounded up to 200 ppb.*

*Note: The *CC* is rounded up to one significant digit to be conservative, and because the safety factor is one significant digit.

Step 2. Estimation Of Surface Water Concentrations

Now that a freshwater *CC* for Chemical A (200 ppb) has been established, the site-specific release can be evaluated. Assume the following:

- Company ABCDE will discharge 200 kg/day of Chemical A for 300 days per year; and
- There will be 50 percent removal of Chemical A in wastewater treatment.
- The fish *BCF* value predicted by EPIWIN is 175 (not the log BCF)

After talking to Company representatives, the assessor has determined that:

- Company ABCDE discharges to the Little Genesee Creek;
- The *NPDES* Number is NY0022381.

Using this information the assessor can use the E-FAST model to calculate: the concentration of Chemical A in the Little Genesee Creek; the potential drinking water exposures; and the potential fish ingestion exposure and the potential risk to the aquatic environment.

CASE STUDY A
Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility (continued)

Run the E-FAST General Population Exposure Module

The following is a step-by-step description of how to run the CEM module.

Once you have entered the E-FAST model:

1. Select: General Population Exposure Module;
2. Enter the chemical identification "Case A", and select 1 Manufacturing Scenario, then click on Continue button.
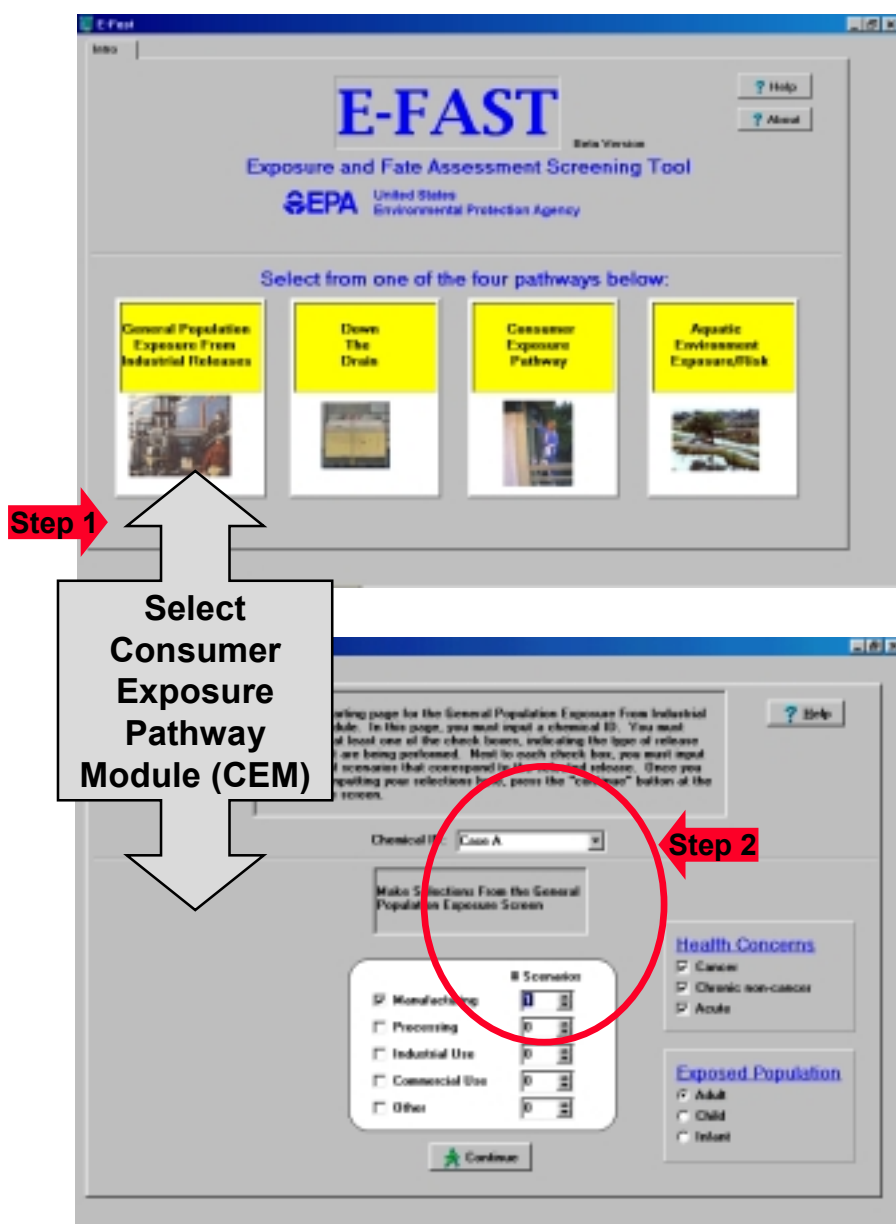
CASE STUDY A
Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility (continued)

Run the E-FAST General Population Exposure Module (continued)

3. You automatically go to the Release Info page. Put a check in the Surface Water box and add Release Amount (200 kg/site/day) and Release Days per Year (300 days/yr)
4. Click on Facility button. You go to the Select a Facility screen.

CASE STUDY A
Potential Aquatic and Human Exposures to Surface
Water Discharges from a Manufacturing Facility (continued)

Run the E-FAST General Population Exposure Module (continued)

5. In the Select a Facility screen, type the *NPDES* number (NY0022381) in the proper box. Click on Perform Search for Facility Button. When the search finds the facility, Double click the facility name. Click on Continue button.

CASE STUDY A
Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility (continued)

Run the E-FAST General Population Exposure Module (continued)

6. You are sent to the Physical Chemical Properties screen, and you should enter the *BCF* (175) and *Concern Concentration* (200 ppb or µg/L). Click on Continue button.

CASE STUDY A
Potential Aquatic and Human Exposures to Surface
Water Discharges from a Manufacturing Facility (continued)

Run the E-FAST General Population Exposure Module (continued)

7. You are sent to the Exposure Factors Screen where you can review the defaults values.
    Any of these can be adjusted as necessary. Click on Continue button.

CASE STUDY A
Potential Aquatic and Human Exposures to Surface
Water Discharges from a Manufacturing Facility (continued)

Run the E-FAST General Population Exposure Module (continued)

8. You are sent to the Fate Properties Screen where you will enter the percent removal in wastewater treatment (enter 50% for both high and low). Click on Calculate, Save Results, and Display Results button.

CASE STUDY A
Potential Aquatic and Human Exposures to Surface
Water Discharges from a Manufacturing Facility (continued)

Run the E-FAST General Population Exposure Module (continued)

9. Environmental Release Results are calculated and you get a message saying the file is
   saved to the A:\ drive. Click on OK. Click on River tab.

CASE STUDY A
Potential Aquatic and Human Exposures to Surface
Water Discharges from a Manufacturing Facility (continued)

Run the E-FAST General Population Exposure Module (continued)

10. Site-Specific Human and Aquatic Exposures to Surface Water Releases - Drinking Water
    Exposure Estimates Results are displayed.   You can click on Fish Ingestion Information to
    view those exposure estimates.

CASE STUDY A
Potential Aquatic and Human Exposures to Surface Water Discharges from a Manufacturing Facility

Run the E-FAST General Population Exposure Module (continued)

11. Click on General Site Information to view Aquatic Exposure Estimates. Click on PDM Site tab to view PDM Site-Specific Aquatic Exposure estimates. Congratulations! You have your results. The *CC* will be exceeded **240 days per year**.

Notes

Case Study B

Potential Exposures to Surface Water Discharges
from a Manufacturing Facility

Uses the Models PCKOCWIN, BIOWIN, KOWWIN,
STPWIN, and ReachScan

CASE STUDY B
Potential Exposures to Surface Water Discharges from a Manufacturing Facility

Introduction

This case study will assess potential drinking water exposures to humans and the presence of endangered species that may be exposed to discharges from a manufacturing facility. The Hamlette Pharmaceutical Manufacturing Company (HPM) is located in Pennsylvania. HPM wishes to use Chemical B in their manufacturing process. HPM discharges to the local POTW, which is upstream from the intake for a downstream community's water treatment plant. Chemical B, which could be toxic to humans at certain concentrations, is a component of the discharge stream going to the POTW. HPM risk assessors wants to estimate the potential exposure of humans to drinking water contaminated with Chemical B as a result of *effluent* discharge from their manufacturing facility, and evaluate the potential presence of endangered species. She will need to run ReachScan, and the KOC (organic carbon sorption coefficient) of the chemical is needed to run ReachScan. Since she does not have a measured KOC, she will run KOCWIN.

The assessor prepares to run the following models:

- KOCWIN to estimate the KOC (organic carbon sorption coefficient) of Chemical B; and

- ReachScan will calculate the stream concentration of Chemical B at the intake pipe of the local water treatment plant. Using the stream concentration, the assessor can calculate the potential human drinking water exposure from Chemical B.

The risk assessor knows the HPM manufacturing plant has an *Indirect Discharge NPDES* permit and pumps discharges to the local POTW. She also knows the following information about the HPM plant:

- Discharge rate = 2000 kg/day;

- Number of release days/year = 150; and

- Discharges are pumped to the West Chester Borough-Goose Creek POTW.

She telephones the POTW manager and receives the following information:

- *NPDES* number of the POTW = PA0027031; and

- Hydrologic region = 02.

CASE STUDY B
Potential Exposures to Surface Water
Discharges from a Manufacturing Facility (continued)

Step 1. Physical / Chemical Property Estimation

Chemical B is an aromatic hydrocarbon (structure at right), and in the neutral organic chemical class. It has the following known physical/chemical properties:
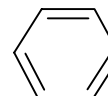
- Molecular weight = 78;

- Water solubility = 1800 *mg/L*; and

- Vapor pressure = 95.3 mm-Hg;

Since the assessor does not have the *CAS Number*, she will write the SMILES notation (shown at right) to run the PCKOCWIN program.
One correct SMILES is c1ccccc1.
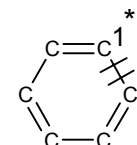
Running PCKOCWIN - The only input required is the SMILES notation which translates the chemical structure into a format understood by computer models. Enter the SMILES notation and the model then calculates a *KOC* value for Chemical B.

PCKOCWIN Results - *KOC* = 165.5 (see Figure B1).

Figure B1
Results of Running PCKOCWIN Model

```
                          Koc (estimated)  :  165
SMILES       :    c1ccccc1
CHEM         :    Chemical B
MOL FOR      :    C6 H6
MOL WT       :    78.11
-------------------------------------------------------------------------------------
         First Order Molecular Connectivity Index ………………………..  :    3.00
         Non-Corrected Log Koc …………………………………………  :    2.2187
         Fragment Correction(s) :      --< NONE
         Corrected Log Koc  ……………………………………………  :    2.2187

                        Estimated Koc  :  165
-------------------------------------------------------------------------------------
```

CASE STUDY B
Potential Exposures to Surface Water
Discharges from a Manufacturing Facility (continued)

Step 2. Estimation Of Surface Water Concentration

The assessor will run ReachScan to predict the concentration of Chemical B in the receiving water after treatment in the POTW. Since she knows the hydrologic region number and *NPDES* number of the receiving POTW she can enter this information into ReachScan to retrieve flow data for the POTW to which HPM discharges. She also knows the likely release amounts, and using this information, she can predict the surface water concentration. She enters ReachScan (Figure B2) then she will go through a series of steps to run the model.

Figure B2
Initial Screen in ReachScan

ReachScan

Methodology and Program Development by

Sidney W. Abel, III	Gerald LaVeck	Keith Drewes
US EPA -	US EPA -	Versar, Inc.
Office of Pollution	Office Water	Exposure Assessment
Prevention and Toxics		Springfield, VA 22151
Washington, DC 20460	Washington, DC 20460	Phone (703) 750-3000
Phone (202) 260-3920	Phone (202) 260-7771	Phone (800) 2-VERSAR

Press any key to continue . . .

Updated : March 9, 1995   Versar, Inc.

CASE STUDY B
Potential Exposures to Surface Water
Discharges from a Manufacturing Facility (continued)

1. Select a Region: Region 02 (see Figure B3)

Figure B3
ReachScan Opening Screen

ReachScan Opening Menu

Select a Region
Change Data File Location
Change Output File Location
Exit ReachScan

Current Data Location: J:\env_ops\common\expmodel\rscanpdm\

F1: Help

Figure B4
Select a Hydrologic Region Screen in ReachScan

Region   01
Region   02
Region   03
Region   04
Region   05
Region   06
Region   07
Region   08
Region   09
Region   10
Region   11
Region   12
Region   13
Region   14
Region   15
Region   16
Region   17
Region   18

CASE STUDY B
Potential Exposures to Surface Water
Discharges from a Manufacturing Facility (continued)

2. Select Search by *NPDES* number (Figure B5), and enter *NPDES* of the POTW: PA0027031

Figure B5
ReachScan Main Menu Screen

```
                    ReachScan Main Menu

  ┌─────────────────────────────────────────────┐
  │                                               │
Step2 ⮞  Begin Search by NPDES Number            │
  │      Begin Search by Facility Name            │
  │      Begin Search by SIC Code                 │
  │      Begin Search by Water Utility Name       │
  │      Begin Search by Reach Number             │
  │      Select Another Region                    │
  │      Change Data File Location                │
  │      Exit ReachScan                           │
  └─────────────────────────────────────────────┘

  ┌─────────────────────────────────────────────┐
  │  Active Region : Region 02                    │
  │  Current Data Location: J:\env_ops\common\expmodel\rscanpdm\ │
  └─────────────────────────────────────────────┘

     F1: Help
```

Figure B6
NPDES Selection Screen - Results of Searching by *NPDES*

```
                        NPDES Selection

  SIC    FACILITY NAME                    NPDES        REACH        KM UP
  4952   WEST CHESTER BOROUGH-GOOSE-CRE   PA0027031    02040205007   3.86




     F1: Help        F9: Back        Total Items --> 1        <Esc>: Exit
```

CASE STUDY B
Potential Exposures to Surface Water
Discharges from a Manufacturing Facility (continued)

3. Search Query (Figure B7):

    • Check for reported presence of endangered species in the county

    • Search: distance of 100 km; downstream; for the presence of a utility

Figure B7
Search Query Screen in ReachScan

CASE STUDY B
Potential Exposures to Surface Water
Discharges from a Manufacturing Facility (continued)

4. Enter Concentration Parameters (Figure B8)

    • Loading (amount released after treatment in kg/day) = 300.0

    • Consider Environmental Fate = Yes (Note: If environmental fate is not considered, the model will calculate the concentration using default values, and the predicted concentration may be higher than the actual value that would be observed.)

    • Select flow type = mean (for drinking water concerns select mean, for aquatic life concerns select low)

Figure B8
Concentration Parameters Screen in ReachScan

CASE STUDY B
Potential Exposures to Surface Water
Discharges from a Manufacturing Facility (continued)

ReachScan Environmental Effects Results - To view endangered species present, press the F7 key when in Environmental Effects Screen.

- Aquatic = none; and
- Terrestrial = Delmarva Peninsula fox squirrel, Indiana bat.

Figure B9
Environmental Effects Screen in ReachScan

```
                         Environmental Effects
                         ─────────────────────

    Region          :  Region 02
    Calc Parameters :  3.00E+02        |    Yes    |     Mean
    Search Parameters :  Down          |   Utility |     100.00

    SIC   Facility Name                    NPDES       Reach        km Up

    4952  WEST CHESTER BOROUGH-GOOSE-CRE   PA0027031   02040205007    3.86

          ┌─────────────────────────────────────────────────────┐
          │ Chemical Name (optional)              Chemical B      │
          │ Molecular Weight (g/mol)              7.80E+01        │
          │ Water Solubility (ppm)                1.80E+03        │
          │ Vapor Pressure (mm-Hg)                9.53E+01        │
          │ Sorption Coefficient                  1.66E+02        │
          │ Chemical half-live due to Degradation (hrs)  3.36E+02 │
          │ Suspended Solids Concentration (ppm)  1.50E+01        │
          └─────────────────────────────────────────────────────┘

          Press <ENTER> to edit parameter.      Use arrow keys to move about.

    F1: Help      F7: Endangered Species      F9: Back      F10: Next      <Esc>: Exit
```

PCKOCWIN Results: KOC = 165.5

Figure B10
Endangered Species Report Screen in ReachScan

```
                         Endangered Species Report
    ...................................................................

    County        :  CHESTER          State :   PA        State FIPS  :   42
                                                          County FIPS :   029
    Inventory Name :  SQUIRREL, DELMARVA PENINSULA FOX
    Scientific Name :  Sciurus niger cinereus
    Common Name   :  Delmarva Peninsula fox squirrel
    Group Name    :  MAMMAL
    Family        :  Sciuridae          Order :   Rodentia
    Status        :   EXN               Action :   1
    Proposed Date :
    Critical Habitat :

    County        :  CHESTER          State :   PA        State FIPS :   42
    ...................................................................  County FIPS  :   029
    Inventory Name :  BAT, INDIANA
    Scientific Name :  Myotis sodalis
    Common Name   :  Indiana bat
    Group Name    :  MAMMAL
    Family        :  Vespertilionidae    Order :   Chiroptera
    Status        :   ECN               Action :   C
    Proposed Date :  75-12-6
    Critical Habitat :  17.92 (a)         ESPP :   N
```

CASE STUDY B
Potential Exposures to Surface Water
Discharges from a Manufacturing Facility (continued)

ReachScan Results - (Figure B11)

- Utility name: Wilmington Water Company
  - Mean stream flow = 1,252 MLD
  - Km downstream from HPM = 30.6 km
  - Population served = 140,000
  - Concentration of Chemical B in the *influent* = 0.26 µg/L

Step 3. Estimation Of Potential Human Drinking Water Exposure

The risk assessor will then estimate the potential exposure from ingesting drinking water contaminated with Chemical B at a concentration of 0.26 µg/L. She assumes an ingestion rate of 2 liters per day. Therefore, the potential exposure is (2 L/day) x (0.26 µg/L) = 0.52 µg/day.

Figure B11
Search Results Screen in ReachScan


```
                          ┌─ Search Results ─┐
 Region            :   Region 02
 Calc Parameters   :   3.00E+02    | Env. Effects:  Y  |        Mean
 Search Parameters :   Downstream  |    Utility        |       100.00

 SIC    Facility Name                          NPDES        Reach              km Up

 4952   WEST CHESTER BOROUGH-GOOSE-CRE    PA0027031     02040205007            3.86

                          MEAN
                 REACH    H FLOW   VEL    KM  DN    POP          V    CONC
 UTILITY NAME    NUMBER   C (MLD)  (M/S)  STREAM    SERVED       C    (µ/l)

 WILMINGTON WATER CO  02040205006  1252.37  0.47   30.6    140000      V    2.61E-01
                      02040205005  2127.21  0.47   37.6         0           3.18E-02
                      02040204060  2139.9   0.47   39.0         0           2.34E-02
                      02040204050  47681.18 1.12   59.4         0           8.34E-05
                      02040204052  N/A      N/A    LEV 0        0           N/A
                      02040204051  N/A      N/A    LEV 0        0           N/A
                      02040204046  48284.90 1.12   66.2         0           2.29E-05
                      02040204048  N/A      N/A    LEV 0        0           N/A
                      02040204047  N/A      N/A    LEV 0        0           N/A
                      02040204042  48338.91 1.12   72.8         0           6.57E-06
                      02040204044  N/A      N/A    LEV 0        0           N/A
                      02040204043  N/A      N/A    LEV 0        0           N/A

   <F1;>Help  <F2>Print    <F3>File    <F9>Back    <F10>Next    <Esc>: Main Menu
```

Case Study C

Consumer Dermal Exposure

Uses the E-FAST
Consumer Exposure Pathway (CEM) Module

Notes

CASE STUDY C
Consumer Exposure from Dermal Contact

Introduction

The purpose of this case study is to assess consumer exposure that may result from dermal contact with a proposed new additive to a consumer product. The Brown Manufacturing Corporation (BMC) is considering using Chemical C as a colorant in a new bar soap product. The BMC risk assessor must estimate potential consumer exposure to Chemical C before BMC product developers can make the decision to proceed with the new formulation. The assessor will use the E-FAST Consumer Exposure Module (CEM) to predict a Potential Lifetime Average Daily Dose (*LADD*) Rate, a Potential Average Daily Dose (*ADD*) Rate, and an Acute Potential Dose Rate (*APDR*) for a consumer from dermal contact with Chemical C in the soap product through hand and body washes.

The BMC risk assessor knows the following information about the proposed product and candidate Chemical C:
   * Weight fraction of Chemical C in the final soap product will be 0.0025 - 0.0075 (percent by weight) (median = 0.005); and
   * The chronic oral RfD for an adult (70 kg average body weight) for Chemical C is 0.02 mg/kg-day.

Estimation Of *APDR*, *ADD* and *LADD* Using CEM

Enter E-FAST (Figure C1). Proceed with the following steps:

1. Select Consumer Exposure Pathway Module (Figure C2);
2. Select Begin New CEM Run (Figure C2);
3. In the CEM Introduction Screen, enter Chemical Identification Information (Figure C3);
4. Click on the Scenario Tab (Figure C3);
5. Choose Bar Soap (Figure C4);
6. Click on Dermal Inputs Tab and view preset defaults (Figure C5). Any of these defaults can be overridden if necessary.
7. Click on Chemical Properties Tab and enter weight fraction information (Figure C6).
   * Median   = 0.005
   * *High end* (90th%)   = 0.0075;
8. Select Run the model (Figure C6).
9. Results are displayed. Click on Outputs-Dermal (Figure C6). Results can be saved in a WP file or printed.

CASE STUDY C
Consumer Exposure from Dermal Contact

CEM Model Results

After running the CEM model, the BMC risk assessor obtained the following predicted exposure results (see Figure C6):

LADD	=	2.71e-03 mg/kg-day
ADD	=	2.75e-03 mg/kg-day
APDR	=	4.52e-03 mg/kg-day

In-house studies have demonstrated that the **dermal absorption fraction** of Chemical C is 10 to 20 percent of the applied dose. Using the more conservative value of 20 percent absorption, the assessor will adjust the predicted ADPR 4.52e-03 mg/kg-day to obtain a predicted absorbed adult *dose* of 8.984e-04 mg/kg-day. This is below the reported adult chronic oral RfD for Chemical C of 2.00e-02 mg/kg-day. The assessor will report to product developers that the amount of Chemical C in the soap formulation will not exceed the chronic oral RfD for Chemical C.

CASE STUDY C
Consumer Exposure from Dermal Contact

Figure C1
E-FAST Opening Screen
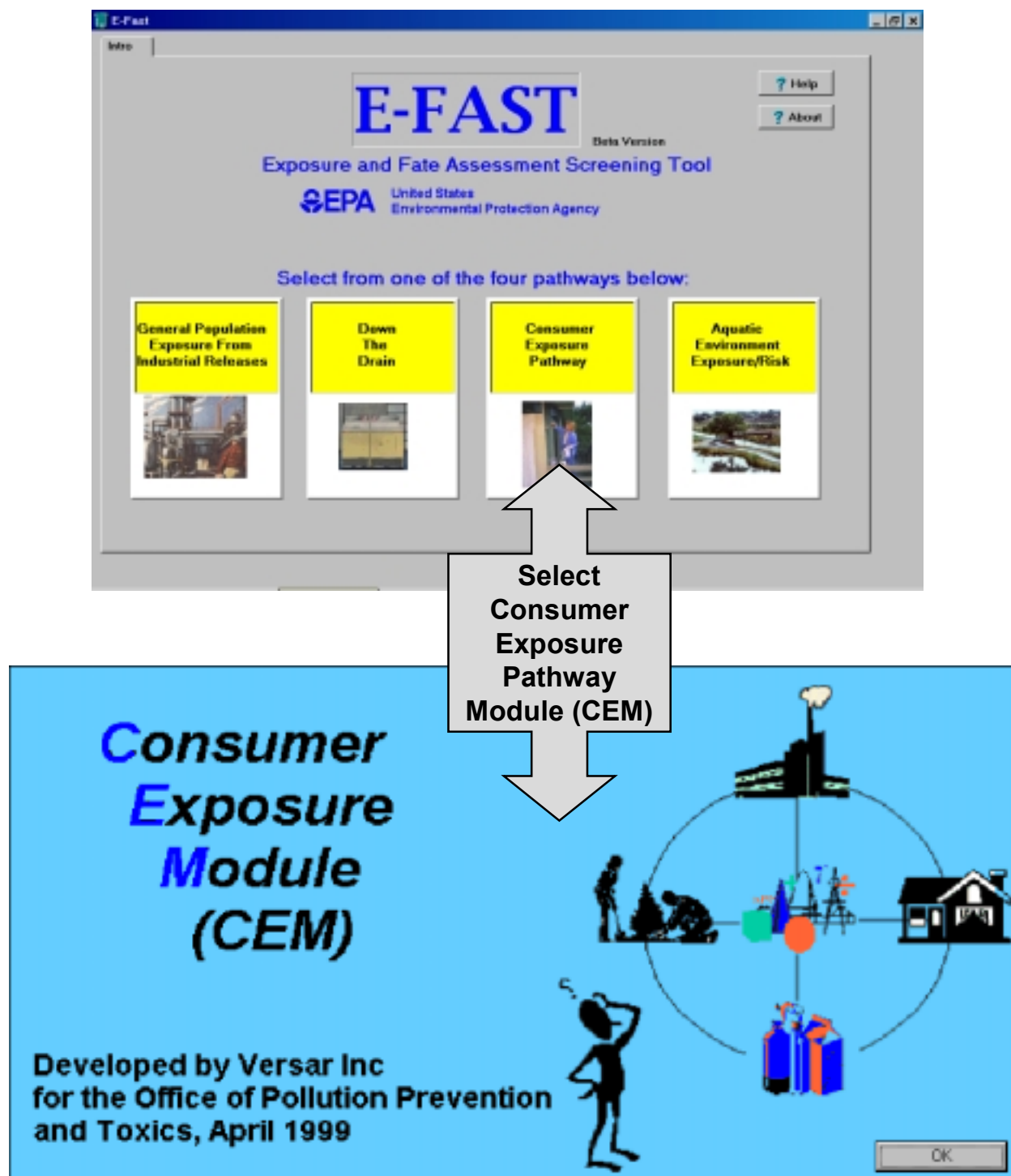
CASE STUDY C
Consumer Exposure from Dermal Contact

Figure C2
CEM Opening Screen
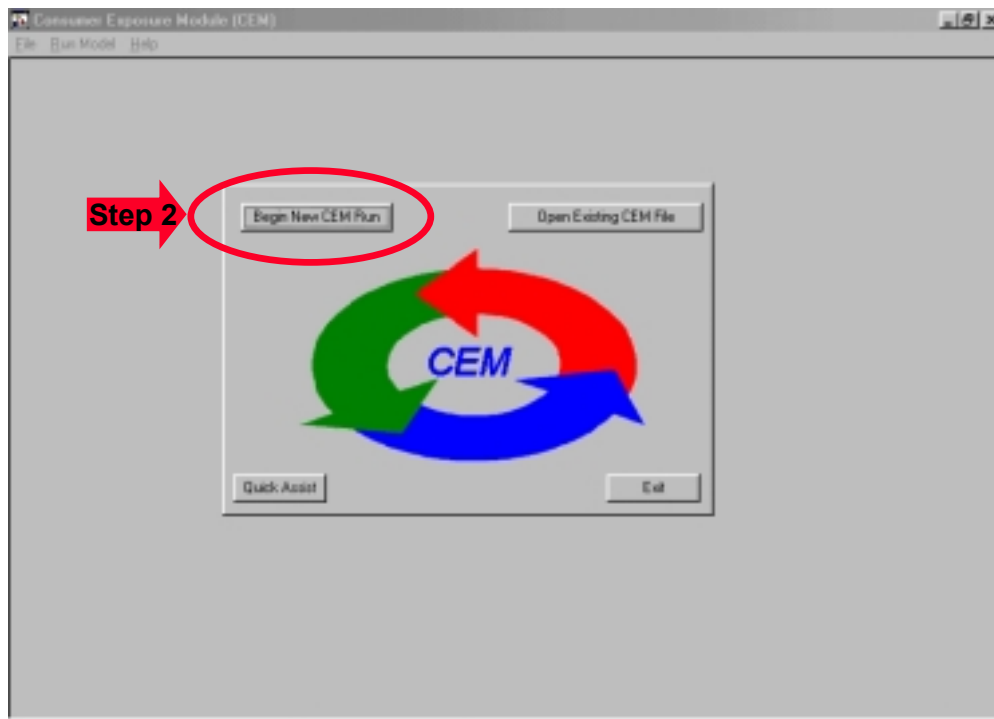
Figure C3
CEM Introduction Screen
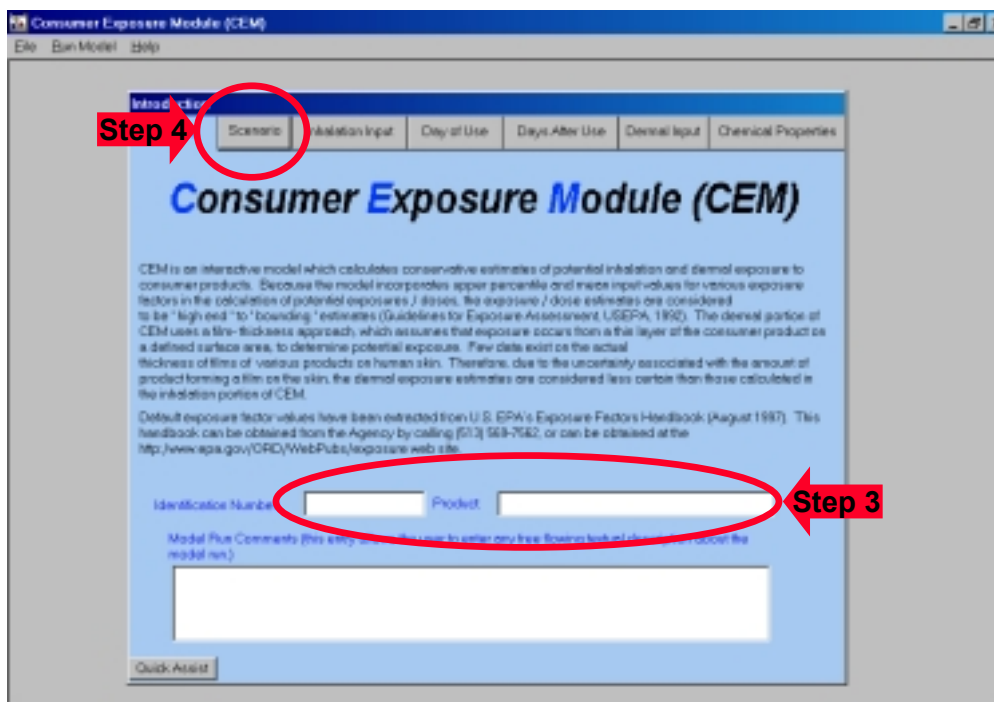
CASE STUDY C
Consumer Exposure from Dermal Contact

Figure C4
Dermal Scenario Selection Screen

Figure C5
Dermal Scenario Input Screen

CASE STUDY C
Consumer Exposure from Dermal Contact

Figure C6
CEM Model Inputs

CASE STUDY C
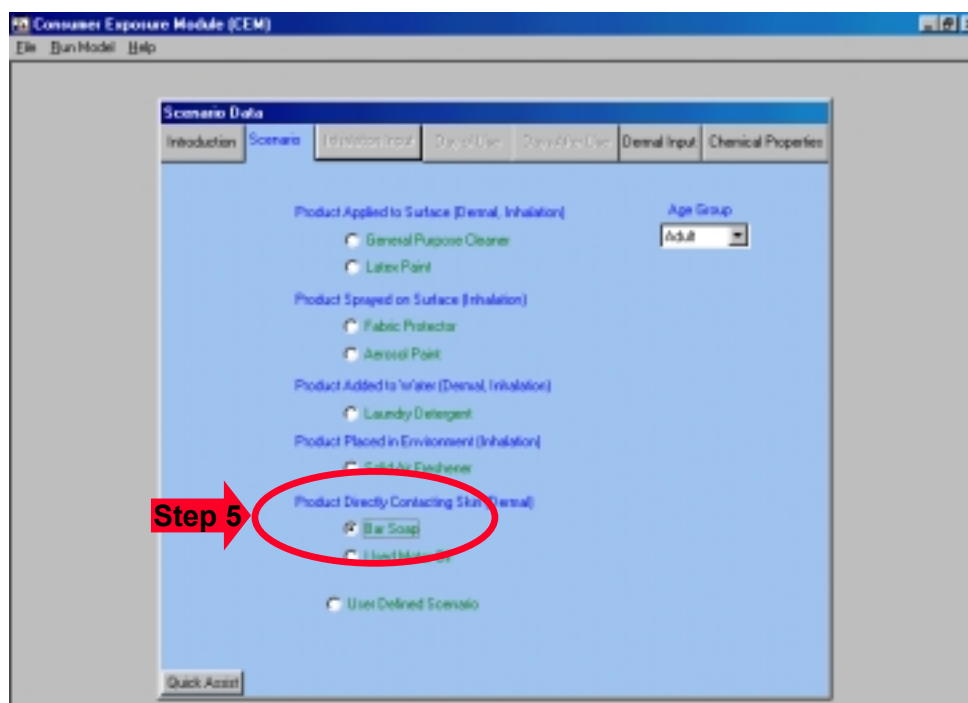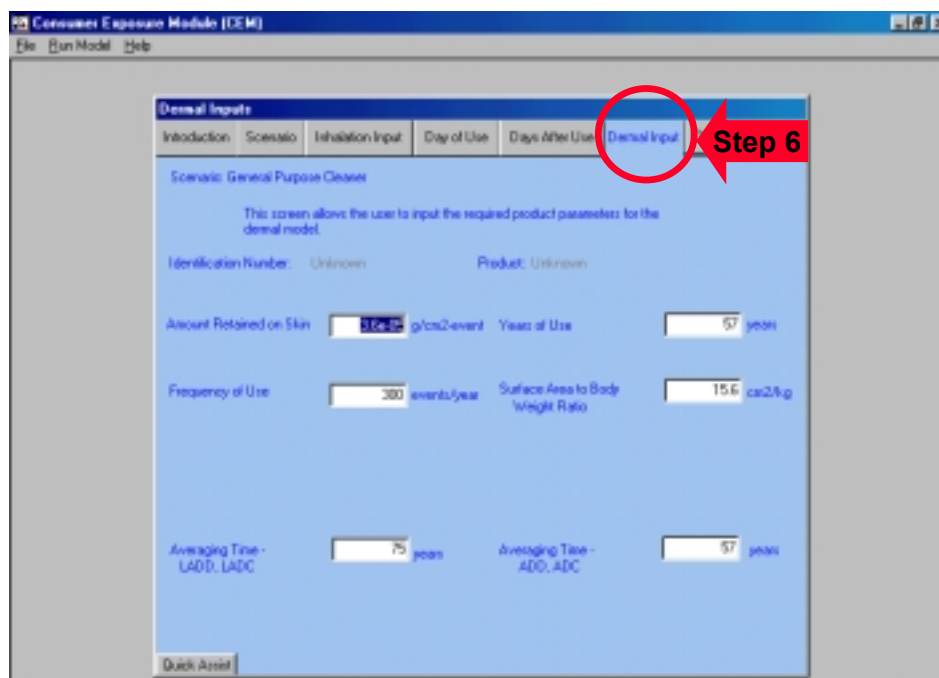## Consumer Exposure from Dermal Contact

Figure C6
CEM Model Results
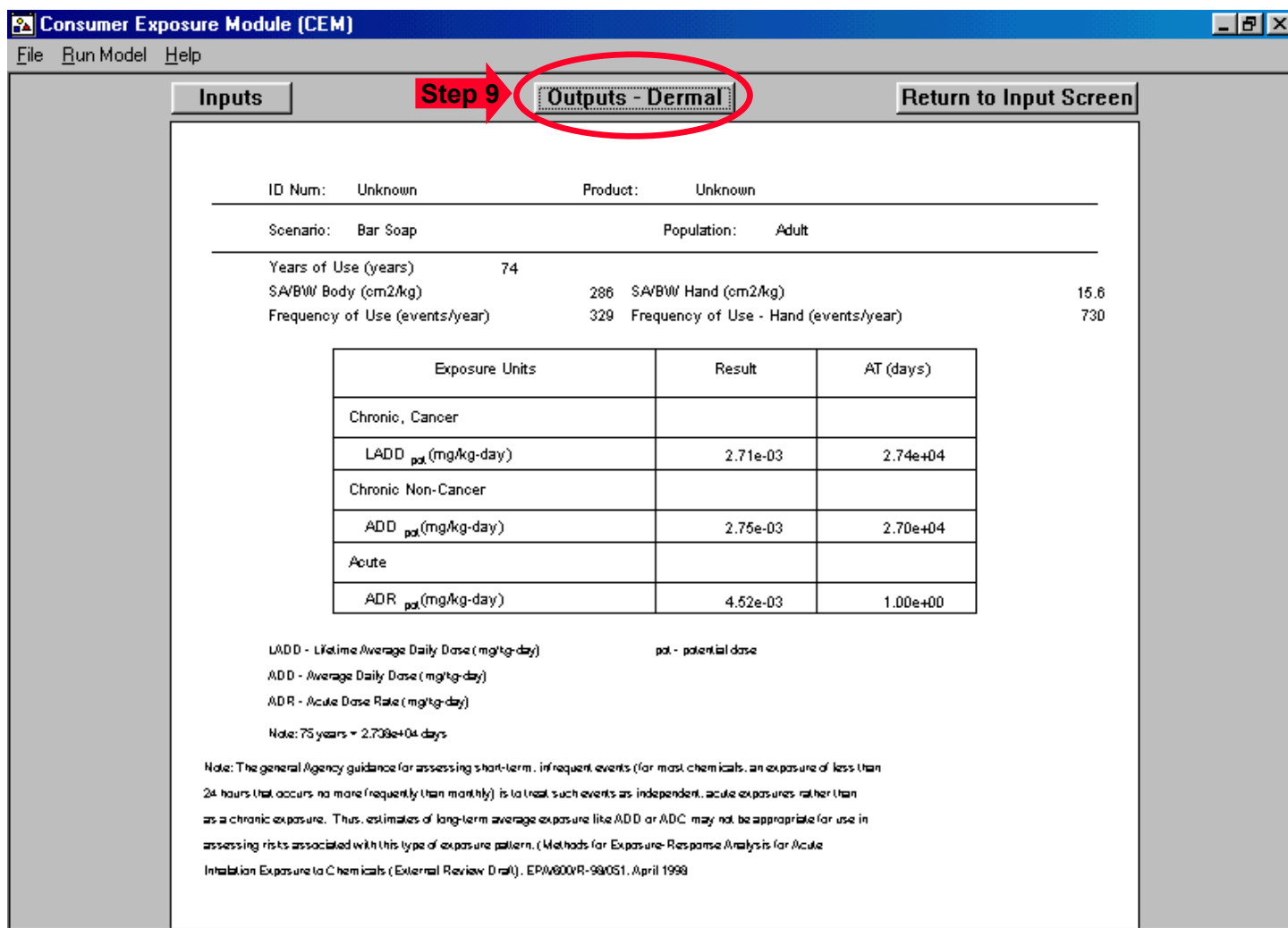
Case Study D

Worker Inhalation Exposure

Uses the Occupational Exposure Spreadsheet

Notes

CASE STUDY D
Worker Inhalation Exposure

Introduction

The purpose of this case study is to assess worker exposure from the inhalation of vapors generated during the transfer/repackaging of a chemical in an industrial setting. The Deal Chemical Company plans to import Chemical D and repackage the chemical for shipment to manufacturers. Deal's risk assessor needs to estimate the potential worker exposures to Chemical D by vapors generated during various transfer/repackaging processes that could be used. The assessor will estimate worker exposure using the Lotus Spreadsheet for Worker Inhalation Exposure. The assessor knows the following information about the chemical and the processes:

- Molecular weight = 250;
- Vapor pressure = 0.1 torr;
- Hours per day of operations = 6; and
- Hours per day of worker exposure = 6.

Estimation Of Worker Inhalation Exposure

Enter the Lotus Spreadsheet for Inhalation Exposure (Figure D1). Enter the required site-specific inputs:

Step 1. Enter the following values in the designated spreadsheet cells :

Molecular weight = 250	cell C6;
Vapor pressure = 0.1 torr	cell C7;
Hours of operation = 6/day	cell C8; and
Hours of worker exposure = 6/day	cell C9.

CASE STUDY D
Worker Inhalation Exposure

Step 2. After entering the specific inputs in Step 1, the spreadsheet automatically calculates predicted worker exposure and vapor generation rates from transfer operations. The results are automatically displayed after data are entered in the proper cells. The spreadsheet is designed to automatically calculate worker exposure from both transfer operations and from sampling and open surface operations. Therefore, the assessor must select the exposure and vapor generation rates appropriate for the specific scenario (i.e., for transfer operations or for sampling and open surface operations).

Results

The results of the calculation for worker exposures from transfer operations are displayed in Figure D2. Worker exposure and vapor generation results are shown (typical and worst case) for drumming, cans/bottles, tank truck and tank car operations.   The inhalation exposures are shown in mg/day, and air concentrations in mg/m3 and ppm. Vapor generation rates are shown in g/sec and kg/day.

CASE STUDY D
Worker Inhalation Exposure

Figure D1

Spreadsheet to Estimate Worker Inhalation Exposure to Vapors from Transfer (Filling) Operations and Open Surfaces (Pools) of Liquid

CEB SPREADSHEET FOR WORKER INHALATION EXPOSURE AND VAPOR GENERATION FROM TRANSFER AND OPEN SURFACE OPERATIONS (1/22/97)
(Uses Cv (eqn 4-14) and vapor generation rate (eqns 4-21 and 4-24) from CEB Eng. Manual)
(Default values are listed in Tables 4-10, 4-11, and 4-12 in CEB Eng. Manual)
REQUIRED, CASE-SPECIFIC INPUTS:

Molecular weight:	**0.00E+00**	
Pure vapor pressure (torr):	**0.00E+00**	These are the four required inputs
Hrs/Day (operations)	**0.00E+00**	
Hrs/Day (worker exposure):	**0.00E+00**	(should be less than or equal to 8)

OTHER REQUIRED INPUTS:

Volumes (cm3):	2.10E+05	Drumming (55 gallons = 2.1E+05 cm3)
	1.90E+04	Cans/bottles (5 gallons = 1.9E+04 cm3)
	1.90E+07	Tank truck (5,000 gallons = 1.9 E+07 cm3)
	7.60E+07	Tank car (20,000 gallons = 7.6E+07 cm3)
Wind Speed (ft/min):	4.40E+02	(average outdoor wind speed = 9 mph (792 ft/min), per CEB Eng. Man. (pg 4-17); average indoor wind speed = 100 ft/min (1.136 mph), per CEB Eng. Man (App. K); 440 ft/min (5 mph) is the CEB default value, per Nhan)
Fill Rates (#/hr)	2.00E+01	Typical cans/drums (20/hr)
	3.00E+01	Worst case cans/drums (30/hr)
	2.00E+00	Typical and worst case tank truck (2/hr)
	1.00E+00	Typical and worst case tank car (1/hr)
Saturation Factors:	5.00E-01	Typical cans/drums (0.5, dimensionless)
	1.00E+00	Worst case cans/drums (1.0, dimensionless)
	1.00E+00	Typical and worst case tank truck/tank car (1.0, dimensionless)
Mixing Factors:	5.00E-01	Typical for all (0.5, dimensionless)
	1.00E-01	Worst case for all (0.1, dimensionless)
Ventilation Rates (ft3/min): 3.00E+03		Typical case cans/drums (3,000 ft3/min)
	5.00E+02	Worst case cans/drums (500 ft3/min)
	1.32E+05	Worst case for tank cars/trucks (ft3/min; dependent on wind speed (26,400*wind speed in mph); NO ENTRY REQUIRED, CALC BASED ON ABOVE WIND SPEED)
	2.38E+05	Typical case for tank cars/trucks (ft3/min; constant based on 9mph, per CEB Eng. Man)
Inhalation Rate (m3/hr):	1.25E+00	Standard inhalation rate (1.25 m3/hr)
Universal Gas Constant:	8.21E+01	R (82.05 atm cm3/gmole K)
Total Pressure (atm):	1.00E+00	(1 atm)
Temperature (K)	2.98E+02	(298 K)
Air Molar Volume (l/gmole)	2.45E+01	(24.45 l/gmole)

CASE STUDY D
Worker Inhalation Exposure

Figure D2

Results from Spreadsheet to Estimate Worker Inhalation Exposure to
Vapors from Transfer (Filling) Operations and Open Surfaces (Pools) of Liquid

Exposure and generation rates from transfer operations can be found at cells E44-E54, and from sampling and open surface at cells D60-D77.

INPUTS	Cell No.
Molecular weight	
250	C6
Vapor pressure	
0.1 torr	C7
Hrs/day operations	
6	C8
Hrs/day worker exposure	
6	C9

RESULTS:

WORKER EXPOSURES AND VAPOR GENERATION RATES FROM TRANSFER OPERATIONS

	Inhalation Exposure			Vapor Generation	
	I[mg/day]	Cm[mg/m^3]	Cv[ppm]	G[g/sec]	G[kg/day]
Drumming (55 gal)					
Worst Case	7.32E+02	9.76E+01	9.54E+00	2.35E-03	5.09E-02
Typical Case	8.13E+00	1.08E+00	1.06E-01	7.85E-04	1.70E-02
Cans/Bottles (5 gal)					
Worst Case	6.62E+01	8.83E+00	8.63E-01	2.13E-04	4.60E-03
Typical Case	7.36E-01	9.81E-02	9.59E-03	7.10E-05	1.53E-03
Tank Truck (5,000 gal)					
Worst Case	1.67E+01	2.23E+00	2.18E-01	1.42E-02	3.07E-01
Typical Case	1.86E+00	2.48E-01	2.42E-02	1.42E-02	3.07E-01
Tank Car (20,000 gal)					
Worst Case	3.34E+01	4.46E+00	4.36E-01	2.84E-02	6.13E-01
Typical Case	3.72E+00	4.95E-01	4.84E-02	2.84E-02	6.13E-01

WORKER EXPOSURES AND VAPOR GENERATION RATES DUE TO SAMPLING AND OPEN SURFACE

	Inhalation Exposure			AREA	DIAMETER			Vapor Generation	
	I[mg/day]	Cm[mg/m^3]	Cv[ppm]	A[cm^2]	z[cm]	Q[ft3/min]	k	G(g/sec)	G(kg/day)
Sampling									
Worst Case	4.47E+01	5.96E+00	5.83E-01	7.85E+01	1.00E+01	5.00E+02	1.00E-01	1.44E-04	3.11E-03
Typical Case	7.48E-01	9.97E-02	9.75E-03	3.85E+01	7.00E+00	3.50E+03	5.00E-01	8.42E-05	1.82E-03
Open surface									
Worst Case	1.24E+03	1.65E+02	1.61E+01	6.58E+03	9.15E+01	5.00E+02	1.00E-01	3.98E-03	8.59E-02
	6.73E+02	8.98E+01	8.78E+00	2.92E+03	6.10E+01	5.00E+02	1.00E-01	2.17E-03	4.68E-02
	2.38E+02	3.17E+01	3.10E+00	7.31E+02	3.05E+01	5.00E+02	1.00E-01	7.66E-04	1.65E-02
	8.41E+01	1.12E+01	1.10E+00	1.83E+02	1.53E+01	5.00E+02	1.00E-01	2.71E-04	5.85E-03
	2.96E+01	3.95E+00	3.86E-01	4.54E+01	7.60E+00	5.00E+02	1.00E-01	9.52E-05	2.06E-03
	1.62E+01	2.16E+00	2.11E-01	2.03E+01	5.08E+00	5.00E+02	1.00E-01	5.21E-05	1.12E-03
	5.72E+00	7.63E-01	7.46E-02	5.07E+00	2.54E+00	5.00E+02	1.00E-01	1.84E-05	3.97E-04
Typical Case	4.12E+01	5.50E+00	5.38E-01	6.58E+03	9.15E+01	3.00E+03	5.00E-01	3.98E-03	8.59E-02
	2.24E+01	2.99E+00	2.93E-01	2.92E+03	6.10E+01	3.00E+03	5.00E-01	2.17E-03	4.68E-02
	7.93E+00	1.06E+00	1.03E-01	7.31E+02	3.05E+01	3.00E+03	5.00E-01	7.66E-04	1.65E-02
	2.80E+00	3.74E-01	3.66E-02	1.83E+02	1.53E+01	3.00E+03	5.00E-01	2.71E-04	5.85E-03
	9.87E-01	1.32E-01	1.29E-02	4.54E+01	7.60E+00	3.00E+03	5.00E-01	9.52E-05	2.06E-03
	5.39E-01	7.19E-02	7.03E-03	2.03E+01	5.08E+00	3.00E+03	5.00E-01	5.21E-05	1.12E-03
	1.91E-01	2.54E-02	2.49E-03	5.07E+00	2.54E+00	3.00E+03	5.00E-01	1.84E-05	3.97E-04

Notes

APPENDIX B

Data Sources

NOTE: Before using these P2 Framework Models, or any screening level models, a thorough search for measured data should be conducted. Measured data should be used if available instead of estimated data because estimation methods, such as these screening models, contain inherent uncertainties.

The Data Sources included here are not intended to represent the only or best sources of data available. Readers are strongly encouraged to conduct their own searches for data.

Internet addresses provided here may have changed from the time of the writing of this document.

Types of Data Sources included here are:

      1.   Physical / Chemical Property Data

      2.   Chemical Human *Hazard* Data

      3.   Chemical Environmental *Hazard* Data

      4.   Release Data

      5.   Exposure and Population Data

Notes

Data Sources

Physical / Chemical Property and Fate Data Sources:

BIOLOG, BIODEG and FATE/EXPOS: New files on microbial degradation and toxicity as well as environmental fate/exposure of chemicals.   Howard P.H.; Hueber, A.E.; Mulesky, B.C.; Crisman, J.S.; Meylan, W.; Crosbie, E.; Gray, D.A.; Sage, G.W.; Howard, K.P.; LaMacchia, A.; Boethling, R.; Troast, R. 1986. Environ. Toxic. Chem. 5:977-988.

CRC Handbook of Chemistry and Physics: A Ready-Reference Book of Chemical and Physical Data, 78th Edition, 1997. David R. Lide (Editor). CRC Press; ISBN: 0849304784. Handbook contains CAS Registry numbers, and chemical and physical properties.

Handbook of Chemical Property Estimation Methods: Environmental Behavior of Organic Compounds, 1990. Warren J. Lyman, William F. Reehl, and David H. Rosenblatt. American Chemical Society; ISBN: 0841217610. Contains methods for estimating density, vapor pressure, water solubility, and other chemical properties relevant to environmental fate.

Handbook of Environmental Data on Organic Chemicals, 3rd Edition, 1997. Karel Verschueren (Editor). John Wiley & Sons; ISBN: 0471286591. An extensive text compiling information on organic products. The data given include physical properties; e.g., formula, physical appearance, molecular weight, melting point, boiling point, vapor pressure, and solubility.

Handbook of Environmental Degradation Rates.   Howard, P.H.; Boethling, R.S.; Jarvis, W.F.; and Meylan, W. 1991. New York: Lewis Publishers, Inc. ISBN: 0873713583.

Handbook of Environmental Fate and Exposure Data for Organic Chemicals. 1989. P.H. Howard (ed.) Vol I. Large Production and Priority Pollutants. SRC Handbooks Series. Lewis Publishers, Chelsea, MI.

Handbook of Environmental Fate and Exposure Data for Organic Chemicals. 1991. P.H. Howard (ed.) Vol III. Pesticides. SRC Handbooks Series. Lewis Publishers, Chelsea, MI.

Handbook of Environmental Fate and Exposure Data for Organic Chemicals. 1990. P.H. Howard (ed.) Vol II. Solvents. SRC Handbooks Series. Lewis Publishers, Chelsea, MI.

Handbook of Environmental Fate and Exposure Data for Organic Chemicals. 1997. P.H. Howard (ed.) Vol V. Solvents III. SRC Handbooks Series. CRC/Lewis Publishers, Boca Raton, FL.

Handbook of Environmental Fate and Exposure Data for Organic Chemicals. 1992. P.H. Howard (ed.) Vol IV. Solvents II. SRC Handbooks Series. Lewis Publishers, Chelsea, MI.

Handbook of Physical Properties of Organic Chemicals.   PHYSPROP. Howard, P.H.; Meylan, W.M. 1997. CRC/Lewis Publishers, Boca Raton, FL. There is also a database version.

Handbook of Property Estimation Methods for Chemicals. 2000. Boethling, R.S. and MacKay, D. Environmental Health Sciences. Lewis Publishers. Washington, D.C.

Data Sources

Physical / Chemical Property and Fate Data Sources (Continued):

Hawley's Condensed Chemical Dictionary, 13th Edition, 1997. Gessner Goodrich Hawley (Editor), and Richard J., Sr. Lewis (Editor). John Wiley & Sons; ISBN: 0471292052. (A CD-ROM version is also available). A compendium of technical data and descriptive information covering many thousand chemicals, including their industrial uses, and trademark names.

Illustrated Handbook of Physical-Chemical Properties and Environmental Fate for Organic Chemicals. Vol I and II. 1992.   MacKay, D.; Shiu, W.Y; and Kuo, C.M. Lewis Publishers. New York.

Kirk-Othmer Concise Encyclopedia of Chemical Technology, 3rd Edition, 1989. Martin Grayson (Contributor), Herman F. Mark, and Donald F. Othmer. John Wiley & Sons; ISBM: 0471517003. (A revised 27 volume set edition is due out Dec. 1998). This is a comprehensive source of chemical information.

The Merck Index: An Encyclopedia of Chemicals, Drugs and Biologicals, 12th Edition. 1996. Chapman & Hall; ISBN: 0911910123. Handbook contains chemical and physical properties, and CAS Registry numbers.

Data Sources

Chemical Human Hazard Data Sources:

Many online sources of information can be used for finding physical/chemical properties and environmental fate data. Some available data sources are as follows:

CHEMEST- Contains data for estimating the properties and chemicals of environmental concern. Available through Technical Database Services, Inc. Additional information is found at http://www.agnic.nal.usda.gov/agdb/chemest.html (fee)

CHEMFATE - CHEMFATE contains evaluated physical property values, rate constants and monitoring concentrations for approximately 1,730 commercially significant compounds available on DATALOG. Available information is found at http://esc.syrres.com/efdb/Chemfate.htm

ChemFinder- Contains synonyms, the structure, and physical chemical properties. Available at http://www.chemfinder.com/

Chemical Categories. Developed under the New Chemicals Program within EPA's Office of Prevention, Pesticides, and Toxic Substances (OPPT), this document includes summaries of chemical categories developed to facilitate the review process of new chemicals (Premanufacture Notices) under TSCA Section 5. It is not intended to be a comprehensive list of all chemical substances. Chemical Categories is available on the Internet at the following address: http://www.epa.gov/opptintr/newchems/chemcat.htm

Chemical Abstracts Service (CAS), a division of the American Chemical Society, provides fee-based online access to databases of chemical information. A useful method of searching is through CAS's Science and Technology Network (STN) that searches numerous databases of chemical information. CAS's Internet address is: http://www.cas.org

CHEMID - Contains chemical names, synonyms, molecular formulas and CAS numbers. Available through Internet Grateful Med at http://igm.nlm.nih.gov/

Health Effects Assessment Summary Tables (HEAST). 1997. U.S. EPA. Contains RfD, RfC, unit risk, and slope factor values for selected chemicals. Available through the National Information Service (NTIS), Doc. Number OERR 9200.6-303 (97-1).

Health Assessment Documents (HAD) U.S. EPA. Reviews health effects of specific chemicals.

HSDB - Hazardous Substance Databank- This is an on-line database containing information on a chemical properties and fate, human and environmental toxicity, environmental fate, regulations, and treatments. This database is available through TOXNET at: http://toxnet.nlm.nih.gov ; through STN International at; and through CCINFOweb at http://ccinfoweb.ccohs.ca/

IRIS (Integrated Risk Information System). U.S. EPA. Reviews studies used in the derivation of RfD, RfC, unit risk, and slope factor values. A web prototype is available on the Internet at the following address: http://www.epa.gov/ngispgm3/iris.

Data Sources

Chemical Human Hazard Data Sources (Continued):

Agency for Toxic Substances and Disease Registry (ATSDR). U.S. Dept. of Health and Human Services, Undated. Toxicological Profiles. Contains toxicological profiles of hazardous chemicals most often found at facilities on CERCLA's National Priority List. http://www.atsdr.cdc.gov/toxpro2.html

National Institute of Occupational Safety and Health (NIOSH). Presents Health Hazard Evaluations and Industry-wide Studies. Contains literature reviews of occupational exposure data, health effects data, and animal studies. Rationale are presented for the derivation of NIOSH exposure levels. www.cdc.gov/niosh/homepage.html

Patty's Industrial Hygiene and Toxicology, Vols. 1-4. John Wiley & Sons. (CD-ROM version is available). Contains toxicology and properties of selected industrial chemicals and classes of chemicals.

PHYSPROP - The Physical Properties Database (PHYSPROP) contains chemical structures, names and physical properties for over 25,070 chemicals. This information is available at the Syracuse Research Corporation (SRC) web site at http://esc-plaza.syrres.com/interkow/PhysProp.htm (fee).

STN International and CCINFOweb also contain information on chemical abstracts, CAS numbers, molecular formulas, reaction information, chemical indexing,etc.

TSCATS. Provides public assess to information submitted to U.S. EPA under the various sections of TSCA (Toxic Substances Control Act). TSCATS is available from several on-line sources (CIS, NLM) or on the Internet at the following address: http://www.rtk.net/www/data/tsc_all.html.

Data Sources

Chemical Environmental Hazard Data Sources:

Acute Toxicity of Organic Chemicals to Fathead Minnows (*Pimephales promelas*), Vols. 1-5. Brooke, L.T., D.J. Call, D.L. Geiger and C.E. Northcott, Eds. 1984-1990. This is a comprehensive source of measured fish toxicity values for a single species (fathead minnows), including fish LC50 data.

Ambient Water Quality Criteria Documents. U.S. EPA. Contains aquatic toxicity values chemicals for which ambient water quality criteria have been developed, and is useful for organic and inorganic compounds.

Aquatic Information Retrieval (AQUIRE) - Contains data extracted from published literature worldwide and from independently compiled data files; includes data on acute and chronic toxicity, bioaccumulation, and sublethal effects data from tests performed on freshwater and saltwater species. AQUIRE is accessible through CIS (Chemical Information System), EPA's Office of Research and Development; and the entire AQUIRE database can be downloaded from http://www.epa.gov/medecotx/data_download/aquire/aquire_ascii_download.htm

Catalog of Teratogenic Agents (CTA) - Emphasizes human data and covers pharmaceuticals, chemicals, environmental pollutants, food additives, household products, and viruses; substances are listed alphabetically, and each entry briefly summarizes research procedures and results. The Catalog is accessible as a database through CIS (Chemical Information System).

Chemical Carcinogenesis Research Information System (CCRIS) - Contains data derived from carcinogenicity, mutagenicity, tumor promotion, and tumor inhibition studies; contains over 7,300 chemical records and is sponsored by the National Cancer Institute. (The database is available through CIS (Chemical Information System) and the National Library of Medicine's TOXNET system.)

CCRIS (Chemical Carcinogenesis Research Information System) - Sponsored by the National Cancer Institute (NCI), CCRIS contains scientifically evaluated data derived from carcinogenicity, mutagenicity, tumor promotion and tumor inhibition tests on some 8000 chemicals.

Chemical Information System (CIS) (fee) - 30 databases concerned with chemicals having an environmental impact or that are regulated in some way. Originally developed by the National Institutes of Health and EPA for managing chemical data and information, CIS is now owned by Oxford Molecular.

ChemID - Maintained by the National Library of Medicine (NLM); serves as an authority file for the identification of chemical substances cited in NLM databases. ChemID is accessible through NLM's Internet Grateful Med (IGM) service.

Data Sources

Chemical Environmental Hazard Data Sources (Continued):

DART (Development and Reproductive Toxicology) and ETICBACK (Environmental Teratology Information Center Backfile) - DART is a bibliographic database covering literature on teratology and other aspects of developmental toxicology. It is managed by NLM and funded by EPA, the National Institute of Environmental Health Sciences (NIEHS), and the National Center for Toxicological Research of the Food and Drug Administration. DART is a continuation of ETICBACK, which contains 49,000 citations to teratology literature published from 1950_1989.

DATALOG - Contains citations for published articles containing data on the environmental fate and the physical_chemical properties of chemicals released into the environment. Available through CIS (Chemical Information System).

Developmental and Reproductive Toxicology (DART) - Contains teratology, developmental and reproductive toxicology data from published literature; is a continuation of ETICBACK (Environmental Teratology Information Center Backfile) database; DART is searchable as a subfile in the TOXLINE database.

Envirofate - Contains summary information from papers published worldwide on the environmental fate and the physical_chemical properties of chemicals released into the environment; chemicals included are those produced annually in excess of one million pounds; available through CIS (Chemical Information System).

EMIC (Environmental Mutagen Information Center) and EMICBACK (Environmental Mutagen Information Center Backfile) - EMIC is a bibliographic database containing some 20,000 citations to literature on chemical, biological, and physical agents that have been tested for genotoxic activity. It is produced by the Oak Ridge National Laboratory (ORNL) and funded by EPA and NIEHS. EMIC covers literature published since 1991. EMICBACK contains over 75,000 citations to literature published from 1950_1990.

Environmental Mutagen Information Center (EMIC) - A bibliographic database on chemicals, biological and physical agents that have been tested for genotoxic activity. EMIC covers publications from 1991 to present; earlier years are covered in EMICBACK; The database can also be searched online through the TOXLINE database and the TOXNET system.

GENE_TOX (Genetic Toxicology) - Contains genetic toxicology test results on over 3,000 chemicals. Selected mutagenicity assay systems and the source literature are reviewed by work panels of scientific experts for each of the test systems under evaluation. The GENE_TOX data bank is the product of these data review activities. Each test system in GENE_TOX has been peer reviewed and is referenced.

Handbook of Environmental Data on Organic Chemicals, 3rd Edition, 1997. Karel Verschueren (Editor). John Wiley & Sons; ISBN: 0471286591. An extensive text compiling information of organic products. The data given include physical properties: e.g., formula, physical appearance, molecular weight, melting point, boiling point, vapor pressure, and solubility.

Data Sources

Chemical Environmental Hazard Data Sources (Continued):

Hazardous Substances Data Bank (HSDB) [Discussed previously in "Physical / Chemical Property And Fate Data Sources"]

Integrated Risk Information System (IRIS) _ http://www.epa.gov/iris Prepared and maintained by EPA, IRIS is an electronic database containing health risk and EPA regulatory information on specific chemicals. IRIS was developed by EPA staff in response to a growing demand for consistent risk information on chemicals substances for use in decision_making and regulatory activities. IRIS is designed for EPA staff, but is also accessible to state and local environmental health agencies. The information in IRIS is intended for EPA staff with extensive training in toxicology, but with some knowledge of health sciences. (IRIS is accessible through the EPA Web site at http://www.epa.gov/iris. The database can also be searched online through the TOXNET system.) List of IRIS Substances _ http://www.epa.gov/docs/ngispgm3/iris/subst/index.html

IRIS (Integrated Risk Information System) - IRIS is an online database built by the EPA and contains EPA *carcinogenic* and non-*carcinogenic* health risk information on over 500 chemicals. The risk assessment data have been scientifically reviewed by groups of EPA scientists and represent EPA consensus.

Merck Index - Encyclopedia of chemicals, drugs, pesticides, and biologically active substances; is available in both print and electronic versions. The online database, which is available through CIS (Chemical Information System) and DIALOG, contains nearly 10,000 records containing references to approximately 30,000 substances, inclusive dates late 19th century to present, updated semi_annually, produced by Merck & Co., Inc.

National Toxicology Program (NTP) conducts toxicity/carcinogenesis studies on agents suspected of posing hazards to human health; data on more than 800 chemical studies are on file. NTP Information is routinely provided to industry and the public on an as requested basis. National Toxicology Program Technical Reports at http://ehis.niehs.nih.gov/ntp/docs/ntp.html (fee). The National Toxicology Program Web site is http://ntp_server.niehs.nih.gov/Main_Pages/Chem_HS.html NIEHS Environmental Health Information Service (EHIS) is http://ehis.niehs.nih.gov/ntp/docs/chem_hs.html (fee)

National Institute for Occupational Safety and Health (NIOSH) - established by the Occupational Safety and Health Act of 1970; is part of the Centers for Disease Control and Prevention (CDC); is the only federal Institute responsible for conducting research and making recommendations for the prevention of work_related illnesses and injuries. NIOSHTIC and RTECS are both produced by NIOSH. www.cdc.gov/niosh/homepage.html

National Library of Medicine - A national libraries of the United States, located on the campus of the National Institutes of Health, it provides a number of services and resources for use by the American public. Fact sheets on NLM's toxicological databases are at http://sis.nlm.nih.gov/tox_chart.htm

Data Sources

Chemical Environmental Hazard Data Sources (Continued):

NIOSHTIC - the National Institute for Occupational Safety and Health's (NIOSH) electronic, bibliographic database of literature in the field of occupational safety and health. NIOSHTIC is updated quarterly and is available on_line and on compact disk from several vendors. Information contained within NIOSHTIC is selected from a number of sources. NIOSHTIC is accessible as a subfile in the TOXLINE database.
http://www.cdc.gov/niosh/nioshtic.html#NTIC4

PHYTOTOX - Contains data from the open literature on the effects of the application of one concentration of a single organic chemical on a particular plant species of chemicals on terrestrial vascular plants. Phytotox is available through CIS (Chemical Information System), as well as through EPA's Office of Research and Development.

Registry of Toxic Effects of Chemical Substances (RTECS) - Contains over 100,000 records covering 1971 to present, quarterly updates, maintained by NIOSH; is a comprehensive database of toxic effects and general toxicology reviews, data on skin and/or eye irritation, mutation, reproductive consequences, and tumorigenicity are provided. Toxic effects are linked to literature citation from both published and unpublished government reports (including unpublished test data from TSCATS, the EPA TSCA test submissions database), and published articles from the scientific literature. RTECS database is available from a number of vendors and can be accessed via the TOXNET system via TELNET.

Structure and Nomenclature Search System (SANSS) - Contains records for more than 500,000 chemicals, is an index to most of the other CIS (Chemical Information System) components/databases as well as to over 100 other important sources of information on environmentally significant chemicals; is a pointer to CIS sources such as RTECS, the Merck Index, and AQUIRE, as well as non_CIS sources such as IARC Monographs, Hazardous Substances Data Bank, and National Toxicology Program studies.

Subchronic Toxicity of Industrial and Agricultural Chemicals to Fathead Minnows (*Pimephales promelas*), Volume 1. S Call, D.J. and D.L. Geiger, Eds. 1992. source of measured fish toxicity values for a single species (fathead minnows), including fish EC50 data.

Syracuse Research Corporation. Summary of TSCA Section 4 Activity, 1993. Summarizes TSCA Section 4 activity by CAS number.

Toxic Substances Control Act Test Submissions (TSCATS) - Submitted by industry to EPA under several provisions of the Toxic Substances Control Act, TSCATS database indexes these submissions, which include unpublished health and safety studies, chemical test data, and substantial risk data submitted to EPA under TSCA sections 4, 8(d), 8(e), and FYI. The actual studies can be purchased from the National Technical Information Service (NTIS) ($) and CIS (Chemical Information System). They can also be viewed on microfiche in the TSCA Non_Confidential Information Center (also known as the TSCA Docket).

Toxicity of Power Plant Chemicals to Aquatic Life. 1973. Presents aquatic toxicity values for organic and inorganic chemicals used by power plant. U.S. Atomic Energy Commission.

Data Sources

Chemical Environmental Hazard Data Sources (Continued):

TOXLINE - the National Library of Medicine's extensive collection of online bibliographic information covering the biochemical, pharmacological, physiological, and toxicological effects of drugs and other chemicals. TOXLINE and its backfile TOXLINE65 together contain more than 2.5 million bibliographic citations, almost all with abstracts and/or indexing terms and CAS Registry Numbers. The information in TOXLINE is taken from secondary sources which formulate the subfiles listed below. Citations with publication year 1980 and older are located in the backfiles.

TOXNET (TOXicology Data NETwork) is a computerized system of files oriented to toxicology and related areas. It is managed by the National Library of Medicine's (NLM) Toxicology and Environmental Health Information Program (TEHIP) and runs on Sun servers in a UNIX_based environment. http://toxnet.nlm.nih.gov

TOXNET Web interface also allows users to search for toxicology data in the following toxicology data files: Hazardous Substances Data Bank, Chemical Carcinogenesis Research Information System, Integrated Risk Information System, and GENE_TOX, as well as EPA's Toxics Release Inventory (TRI).

Data Sources

Environmental Release Data Sources:

AIRS (Aerometric Information Retrieval System) is the national repository for information about airborne pollution in the United States. There are seven "criteria pollutants" for which data must be reported to EPA and stored in AIRS: PM 10 (particulate matter less than 10 microns in size), carbon monoxide, sulfur dioxide, nitrogen dioxide, lead, reactive volatile organic compounds (VOC), and ozone. http:/www.epa.gov/enviro/

Chemical Engineering Branch Manual for the Preparation of Engineering Assessments. 1991. U.S. EPA. Conducted by IT Environmental Programs for Office of Toxic Substances (OTS) under Contract No. 68-D8-0112. Washington D.C.

ISDB (Industry Studies Database).   U.S. EPA. Contains survey data collected by the Office of Solid Waste (OSW) covering both RCRA and non-RCRA wastes generated by 470 facilities in 11 industries. The data include company identify and location, SIC code, product name, production volume, waste stream properties and category, constituents and their concentrations in the waste stream, management practice and location, and quantity of waste stream.

Kirk-Othmer Concise Encyclopedia of Chemical Technology, 3rd Edition, 1989. Martin Grayson (Contributor), Herman F. Mark, and Donald F. Othmer. John Wiley & Sons; ISBN: 0471517003. This is a comprehensive source of chemical synthesis processes.

NATICH (Nation Air Toxics Information Clearing House) data base. This is an air pollution data based on air permits issued by state and local agencies is available.

Office of Water Effluent Limitations Guidelines and Standards (for selected industries).

PCS (The Permit Compliance System) is an information management system maintained by the U.S. EPA's Office of Wastewater Enforcement and Compliance (OWEC), to track the permit, compliance, and enforcement status of facilities regulated by the National Pollutant Discharge Elimination System (NPDES). PCS tracks information about wastewater treatment, industrial, and Federal facilities discharging into navigable waters. http:/www.epa.gov/enviro/

TRI (Toxic Chemical Release Inventory) Files - TRI contains information on the annual estimated releases of toxic chemicals to the environment. It is mandated by the Emergency Planning and Community Right_to_Know Act and is based upon data submitted to the Environmental Protection Agency (EPA) from industrial facilities throughout the U.S.A. This data includes names and addresses of the facilities, and the amounts of certain toxic chemicals they release to the air, water, or land, or transfer to waste sites. Information is included on over 600 chemicals and chemical categories. Separate TRI files are available for each year beginning with 1987. Since 1991, pollution prevention data are also reported by each facility for each chemical. http:/www.epa.gov/enviro/

Published chemical monitoring data reports.

Company product literature.

Data Sources

Exposure Parameter Data Sources:

Exposure Factors Handbook. 1996. Exposure Factors Handbook: V.I General Factors EPA/600/P-95/002Ba; V.II Food Ingestion Factors EPA/600-P-95/002Bb; V.III Activity Factors EPA/600/P-95-002Bc August 1996. U.S. EPA. Presents a summary of available data on human behaviors and characteristics which affect exposure to environmental contaminants and presents recommended values to use for these factors. It provides factor data on ingestion rates of foods, water, breast milk, and soil; factors for inhalation and dermal exposure; data for body weight, lifetime, activity factors; data for use of consumer products; and data for exposures that occur in residences. Available on the EPA web site in pdf format at: http://www.epa.gov/ORD/WebPubs/exposure/

Methods for Assessing Exposure to Chemical Substances. U.S. EPA. 1985. Office of Toxic Substances (OTS). Prepared by Versar, Inc. under EPA Contract No. 68-01-6271. Washington DC. These methods described in these volumes were identified by OTS (now officially OPPT) as having utility in exposure assessments on existing and new chemicals under the OTS program. The title of the basic volumes are as follows*:

- V. 1. Methods for Assessing Exposure to Chemical Substances. (EPA 560/5-85-001).
- V. 2. Methods for Assessing Exposure to Chemical Substances in the Ambient Environment. (EPA 560/5-85-002).
- V. 3. Methods for Assessing Exposure from Disposal of Chemical Substances (EPA 560/5-85-003).
- V. 4. Methods for Enumerating and Characterizing Populations Exposed to Chemical Substances (EPA 560/5-85-003).
- V. 5. Methods for Assessing Exposure to Chemical Substances in Drinking Water (EPA 560/5-85-005).
- V. 6. Methods for Assessing Occupational Exposure to Chemical Substances (EPA 560/5-85-006).
- V. 7. Methods for Assessing Consumer Exposure to Chemical Substances (EPA 560/5-85-007).
- V. 8. Methods for Assessing Environmental Pathways of Food Contamination (EPA 560/5-85-008).
- V. 9. Methods for Assessing Exposure to Chemical Substances Resulting from Transportation-Related Spills (EPA 560/5-85-009).
- V. 11. Methods for Estimating the Migration of Chemical Substances from Solid Matrices (EPA 560/5-85-015).
- V. 13. Methods for Estimating Retention of Liquids on Hands (EPA 560/55-85-017).

*Volumes 10 and 12 were not issued.

Population Data Sources:

Census of Population Reports. U.S. Bureau of the Census. Available from the U.S. Bureau of the Census on CD-ROM and on the Internet. Populations are characterized geographically by social and economic characteristics, and also by housing characteristics.

Methods for Enumerating and Characterizing Populations Exposed to Chemical Substances. Volume 4. U.S. EPA. Presents methods and data sources for identifying and characterizing populations of interest.

Notes

APPENDIX C

Summary of
Writing
SMILES Notations

SMILES is "Simplified Molecular Input Line Entry System," which translates a chemical's structure into a string of symbols that is easily understood by computer software. SMILES notation are used to enter chemical structure into EPIWIN estimation programs and ECOSAR. Additional examples of SMILES notations are available in the HELP files of EPIWIN and ECOSAR. Software programs are available which can translate a chemical structure into SMILES.
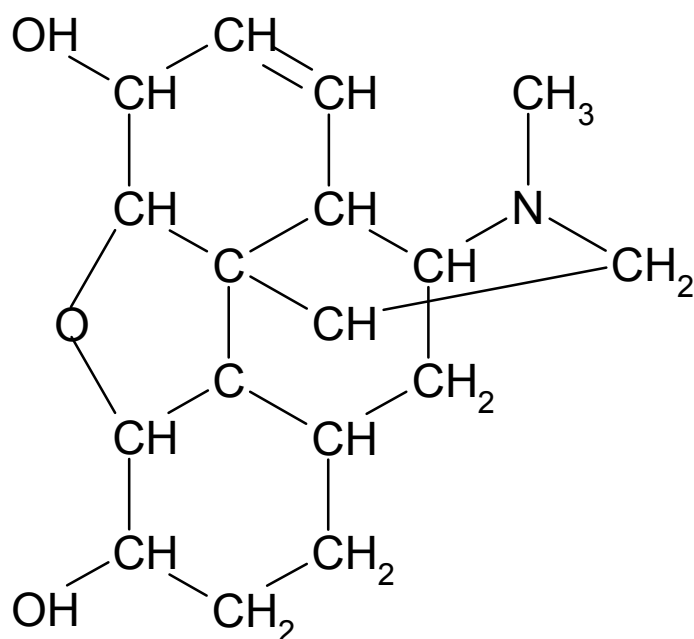
References:

Weininger, D. 1988. SMILES, a Chemical and Information System. 1. Introduction to Methodology and Encoding Rules. J. Chem. Inf. Comput. Sci. 28(1): 31-6.

Wiswesser, W.J. 1954. A Line-Formula Chemical Notation. New York: Cromwell.

SMILES
(Simplified Molecular Input Line Entry System)

The purpose of SMILES is to go from this...

…… to this.

O1C2C(O)C=CC3C2(C4)c5c1c(O)ccc5CC3N(C)C4

SMILES
(Simplified Molecular Input Line Entry System)

Representing Atoms

Atomic symbols and their corresponding SMILES notations:

C	methane (CH_4)
N	ammonia (NH_3)
O	water (H_2O)
P	phosphine (PH_3)
S	hydrogen sulfide (H_2S)
Cl	hydrogen chloride (HCl)

Elements must be described in brackets:

[Au]   elemental gold

SMILES
(Simplified Molecular Input Line Entry System)

Representing Bonds

Single, double, triple, and aromatic bonds are represented by the following symbols:

single	-	triple	#
double	=	aromatic	:

Examples are:

CC	ethane (CH_3CH_3)
C=C	ethylene ($CH_2=CH_2$)
COC	dimethyl ether (CH_3OCH_3)
CCO	ethanol (CH_3CH_2OH)
C=O	formaldehyde (CH_2O)
O=C=O	carbon dioxide (CO_2)
O=CO	formic acid (HCOOH)
C#N	hydrogen cyanide (HCN)
[H][H]	molecular hydrogen (H_2)

Normally single bonds and aromatic bonds do not need to be written in the SMILES notation.

SMILES
(Simplified Molecular Input Line Entry System)

Bonds in Linear Structures

For linear structures, SMILES notation corresponds to conventional diagrammatic notation except that hydrogen can be omitted. For example, there are three correct ways to represent:

6-hydroxy-1,4-hexadiene

> structure: $CH_2=CH-CH_2-CH=CH-CH_2-OH$

> valid SMILES:
> C=CCC=CCO
> C=C-C-C=C-C-O
> OCC=CCC=C

SMILES
(Simplified Molecular Input Line Entry System)

Representing Branches

Branches are specified by enclosures in parentheses, for example:
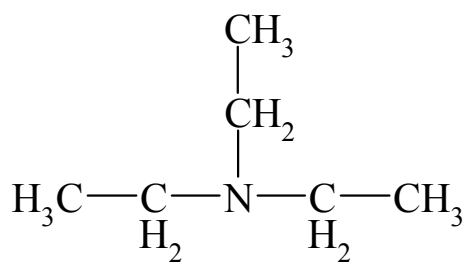
CCN(CC)CC

triethylamine
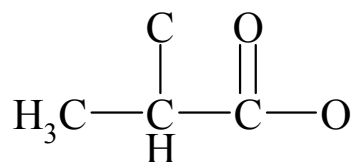
CC(C)C(=O)O

isobutyric acid

SMILES
(Simplified Molecular Input Line Entry System)

Representing Branches

Branches also can be nested or stacked, for example:

$$CH_3$$
$$|$$
$$CH_2 \quad CH_3$$
$$| \qquad |$$
$$CH_2 \quad CH-CH_3$$
$$| \qquad |$$
$$H_2C{=}C{-}C{-}C{-}C{-}C{-}CH_3$$
$$H \quad H \quad H \quad H_2 \quad H_2$$

C=CC(CCC)C(C(C)C)CCC
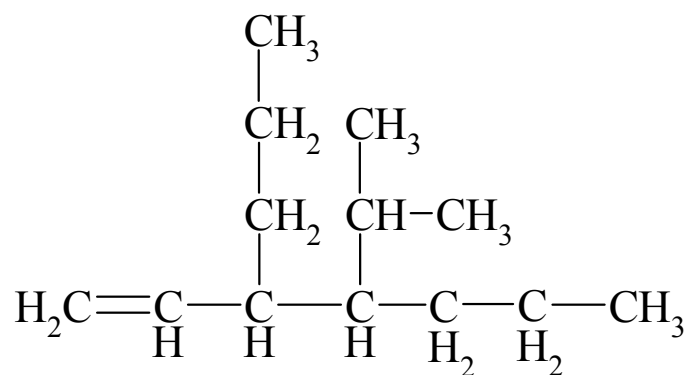
3-propyl-4-isopropyl-1-heptene

SMILES
(Simplified Molecular Input Line Entry System)

Representing Cyclic Structures

Cyclic structures are represented by breaking one single or aromatic bond in each ring. The bonds are numbered in any order, designating ring-opening/closure bonds by a digit immediately following the atomic symbol at each ring closure. This leaves a connected noncyclic graph, which is written as a noncyclic structure by using the three rules described for atoms, bonds, and branches. A typical example is:

cyclohexane

$$\Rightarrow \quad \text{C1CCCCC1}$$
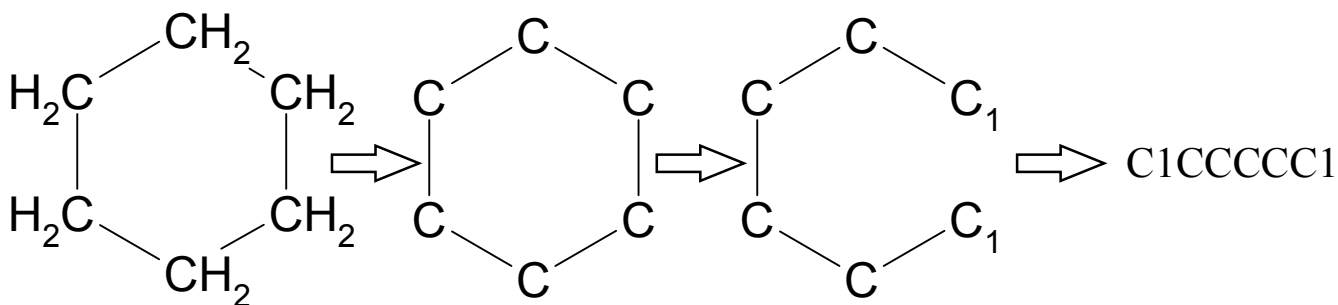
SMILES
(Simplified Molecular Input Line Entry System)

Representing Cyclic Structures

Usually there are many different but equally valid descriptions of the same structure, for example, the following SMILES notations for

1-methyl-3-bromo-cyclohexene

(a)
CC1=CC(Br)CCC1

(b)
CC1=CC(CCC1)Br
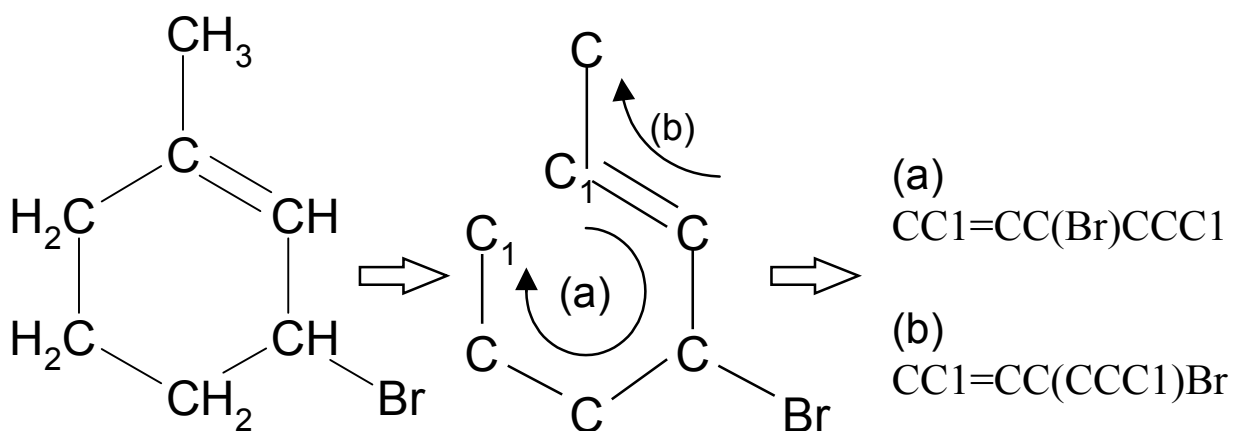
Many other SMILES notations may be written for the same structure from different ring closures.

SMILES
(Simplified Molecular Input Line Entry System)

Representing Cyclic Structures

A single atom may have more than one ring closure. An example of this is cubane, in which two atoms have more than two ring closures.

The generation of the SMILES notation for cubane:

C12C3C4C1C5C4C3C25
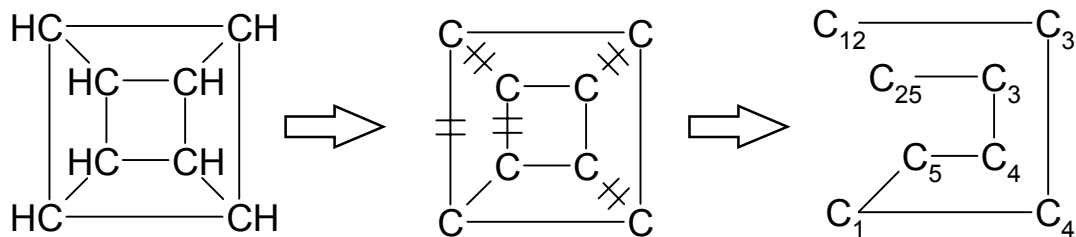
SMILES
(Simplified Molecular Input Line Entry System)

Evolution of SMILES for Morphine
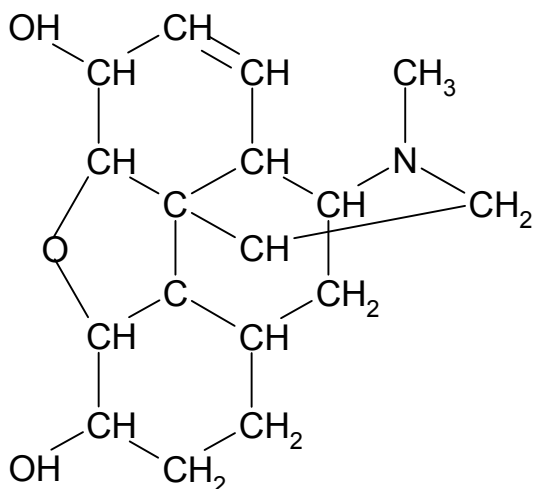
Morphine: Break and number 5 ring closures:
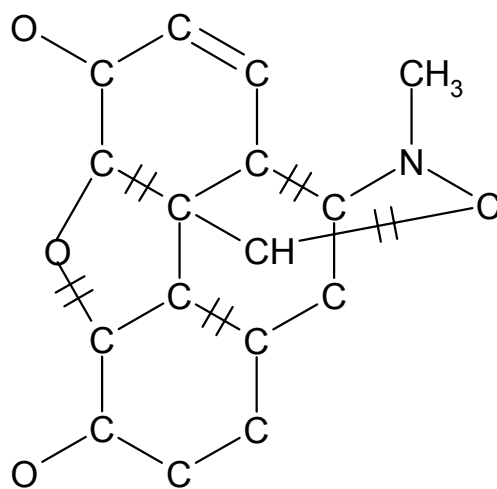
Generate SMILES for the resulting non-cyclic structure by starting at the * and following along the string to the arrow.:
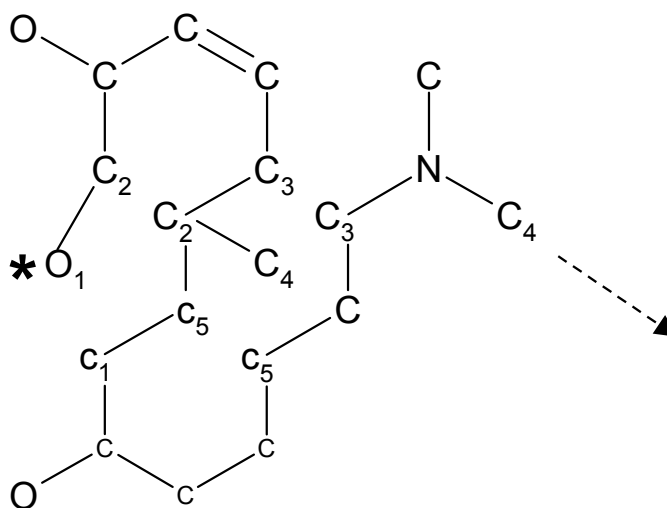
O1C2C(O)C=CC3C2(C4)c5c1c(O)ccc5CC3N(C)C4

SMILES
(Simplified Molecular Input Line Entry System)

Disconnected Structures

Disconnected compounds are written as individual structures separated by a period. The order in which ions or ligands are listed is arbitrary. There is no implied paring of one charge with another, and it is not necessary to have a net charge of zero. If desired, the SMILES of one ion may be imbedded in another, as shown in the example of:

sodium phenoxide
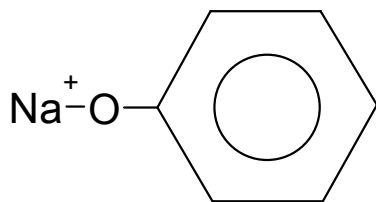
[Na+].[O-]c1ccccc1

or

c1cc([O-].[Na+])ccc1

SMILES
(Simplified Molecular Input Line Entry System)

Aromaticity

Aromatic structures may be distinguished by writing the atoms
in the aromatic ring in lower case letters, for example:

benzoic acid

c1ccccc1C(=O)O
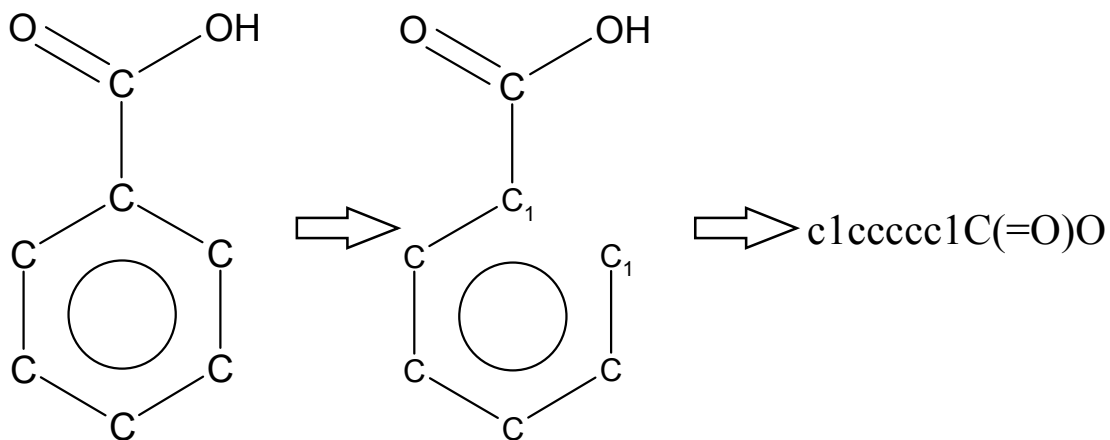
SMILES
(Simplified Molecular Input Line Entry System)

Compounds Containing
Aromatic Nitrogen

To avoid confusion aromatic nitrogens require special attention. There are two types of aromatic nitrogens that are distinguished within the SMILES system. Both types may be specified with the aromatic symbol "n." Examples are pyridine and pyrrole:
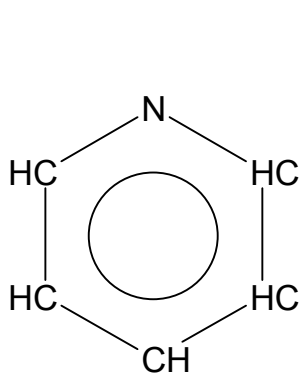
n1ccccc1

O=n1ccccc1   [O-][N+]c1ccccc1
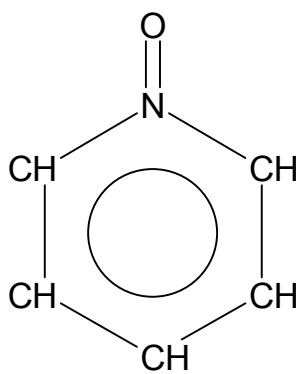
pyridine   pyridine-N-oxide
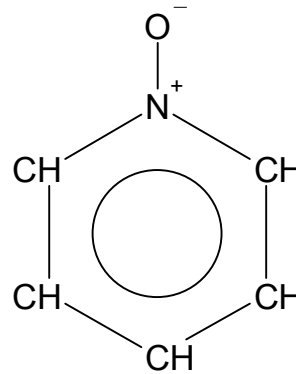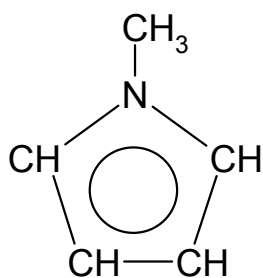
Cn1ccccc1   and   [nH]1ccccc1
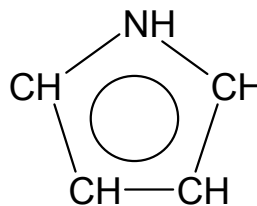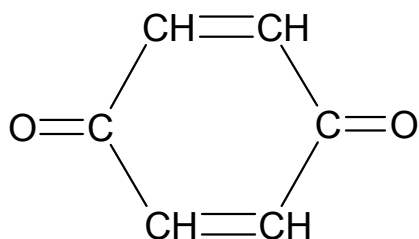
methyl pyrrole   1H-pyrrole

SMILES
(Simplified Molecular Input Line Entry System)

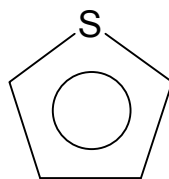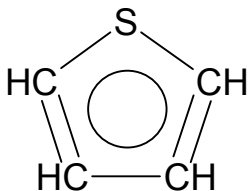## Examples of Aromatic and Nonaromatic Compounds
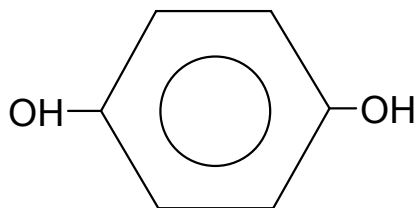
O=c1ccc(O)cc1

Hydroquinone

O=C1C=CC(=O)C=C1

Quinone

In-ring oxygen and sulfur atoms donate a single pair, for example, thiophene:

s1cccc1

Thiophene

Notes